

LIST OF U.S. CUSTOMS LABORATORY METHODS

USCL NUMBER	METHOD	TITLE
27-01	ASTM D 287	<u>Test Method for API Gravity of Crude Petroleum and Petroleum Products (Hydrometer Method)</u>
27-02	ASTM D 1298	<u>Practice for Density, Relative Density (Specific Gravity), or API Gravity of Crude Petroleum and Liquid Petroleum Products by Hydrometer Method</u>
27-03	ASTM D 4006	<u>Test Method for Water in Crude Oil by Distillation</u>
27-04	ASTM D 95	<u>Test Method for Water in Petroleum Products and Bituminous Materials by Distillation</u>
27-05	ASTM D 4928	<u>Test Method for Water in Crude Oils by Coulometric Karl Fischer Titration</u>
27-06	ASTM D 473	<u>Test Method for Sediment in Crude Oils and Fuel Oils by the Extraction Method</u>
27-07	ASTM D 4807	<u>Test Method for Sediment in Crude Oil by Membrane Filtration</u>

USCL NUMBER	METHOD	TITLE
27-08	ASTM D 86	<u>Test Method for Distillation of Petroleum Products</u>
27-09	ASTM D 4953	<u>Test Method for Vapor Pressure of Gasoline and Gasoline-Oxygenate Blends (Dry Method)</u>
27-10	ASTM D 323	<u>Test Method for Vapor Pressure of Petroleum Products (Reid Method)</u>
27-11	ASTM D 445	<u>Test Method for Kinematic Viscosity of Transparent and Opaque Liquids (the Calculation of Dynamic Viscosity)</u>
27-12	ASTM D 88	<u>Test Method for Saybolt Viscosity</u>
27-13	ASTM D 4294	<u>Test Method for Sulfur in Petroleum Products by Energy-Dispersive X-Ray Fluorescence Spectroscopy</u>
27-14	ASTM D 2622	<u>Test Method for Sulfur in Petroleum Products (X-Ray Spectrographic Methods)</u>
27-15	ASTM D 3437	<u>Practice for Sampling and Handling Liquid Cyclic Products</u>
27-16	ASTM E 300	<u>Practice for Sampling Industrial Chemicals</u>
27-17	ASTM D 3438	<u>Practice for Sampling and Handling Naphthalene, Maleic Anhydride, and Phthalic Anhydride</u>

USCL NUMBER	METHOD	TITLE
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27-18	ASTM D 3852	<u>Practice for the Sampling and Handling Phenol and Cresylic Acid</u>
27-19	ASTM D 3439	<u>Test Methods for Assay of Alkaline Cresylate Solutions from Petroleum Sources</u>
27-20	ASTM D 4057	<u>Practice for Manual Sampling of Petroleum and Petroleum Products</u>
27-21	ASTM D 4177	<u>Practice for the Automatic Sampling of Petroleum and Petroleum Products</u>
27-22	ASTM D 396	<u>Specification for Fuel Oils</u>
27-23	ASTM D 975	<u>Specification for Diesel Fuel Oils</u>
27-24	ASTM D 2069	<u>Specification for Marine Fuels</u>
27-25	ASTM D 2880	<u>Specification for Gas Turbine Fuel Oils</u>
27-26	ASTM D 4814	<u>Specification for Automotive Spark-Ignition Engine Fuel</u>
27-27	ASTM D 1655	<u>Specification for Aviation Turbine Fuels</u>
27-28	ASTM D 910	<u>Specification for Aviation Gasolines</u>

USCL NUMBER

METHOD

TITLE

27-29	ASTM D 3699	<u>Specification for Kerosine</u>
27-30	ASTM D 235	<u>Specification for Mineral Spirits (Petroleum Spirits) (Hydrocarbon Dry Cleaning Solvent)</u>
27-31	ASTM D 3735	<u>Specification for VM&P Naphthas</u>
27-32	ASTM D 938	<u>Test Method for Congealing Point of Petroleum Waxes Including Petrolatum</u>
27-33	ASTM D 5	<u>Test Method for Penetration of Bituminous Materials</u>
27-34	ASTM D 217	<u>Test Methods for Cone Penetration of Lubricating Grease</u>
27-35	ASTM D 937	<u>Test Method for Cone Penetration of Petroleum</u>
27-36	ASTM D 1265	<u>Practice for Sampling Liquefied Petroleum (LP) Gases (Manual Method)</u>
27-37	ASTM E 137	<u>Practice for Evaluation of Mass Spectrometers for Quantitative Analysis from a Batch Inlet</u>
27-38	ASTM D 2650	<u>Test Method for Chemical Composition of Gases by Mass Spectrometry</u>
27-39	ASTM D 721	<u>Test Method for Oil Content of Petroleum Waxes</u>

USCL NUMBER

METHOD

TITLE

27-40	ASTM D 140	<u>Practice for Sampling Bituminous Materials</u>
27-41	ASTM D 977	<u>Specification for Emulsified Asphalt</u>
27-42	ASTM D 244	<u>Test Methods for Emulsified Asphalts</u>
27-43	ASTM D 2026	<u>Specifications for Cutback Asphalt (Slow Curing Type)</u>
27-44	ASTM D 2027	<u>Specifications for Cutback Asphalt (Medium Curing Type)</u>
27-45	ASTM D 2028	<u>Specifications for Cutback Asphalt (Rapid Curing Type)</u>
27-		<u>To be assigned</u>
27-47	USCL Manual	<u>Guidelines for Country-of-Origin Determinations of Distillate Petroleum Products from Iraq</u>

U.S. CUSTOMS LABORATORY METHODS

ASTM D 287
Test Method for API Gravity of crude Petroleum and
Petroleum Products (Hydrometer Method)

also an important factor that determines the quality of crude oils.

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method covers the determination by glass hydrometer of the API gravity of crude petroleum and petroleum products normally handled as liquids and having a Reid vapor pressure of 26 psi or less. The API gravity is measured at a given temperature and converted to values at 60°F by means of standard tables.

This method is applicable in the classification of crude petroleum oils and crude oils obtained from bituminous minerals (e.g., from shale, calcareous rock, sand). Crude petroleum oils and crude oils are classifiable according to their API gravity under the tariff heading of HTSUS 2709. Accurate determination of the API gravity of crude petroleum oils and petroleum products is necessary for conversion of

measured volumes to volumes at the standard temperature of 60°F. API gravity is

2 REFERENCES

ASTM D 287

Test Method for API Gravity of Crude Petroleum and Petroleum Products (Hydrometer Method)

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-02

Index

ASTM D 1298

Practice for Density, Relative Density (Specific Gravity), or API Gravity of Crude Petroleum and Liquid Petroleum Products by Hydrometer Meter

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method covers the laboratory determination, using a glass hydrometer, of the density, relative density (specific gravity), or API gravity of crude petroleum, petroleum products, or mixtures of petroleum and non-petroleum products normally handled as liquids, and having a Reid vapor pressure 26 psi or less. Values are measured on a hydrometer at temperatures, readings of density being reduced to 15°C, and readings of relative density (specific gravity) and API gravity to 60°C, by means of international standard tables.

This method is applicable in the classification of crude petroleum oils and crude oils obtained from bituminous

minerals (e.g., from shale, calcareous rock, sand). Crude petroleum oils and crude oils are classifiable according to their API gravity under the tariff heading of HTSUS 2709. Accurate determination of the gravity of crude petroleum oils and crude oils is necessary for the conversion of measured volumes at a measured temperature to volumes at standard temperature of 60°F. API gravity is also an important factor that determines the quality of crude oils.

2 REFERENCES

ASTM D 1298

Practice for Density, Relative Density (Specific Gravity), or API Gravity of Crude Petroleum and Liquid Petroleum Products by Hydrometer Method

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-03

Index

ASTM D 4006

Test Method for Water in Crude Oil by Distillation

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method covers the determination of water in petroleum crude oils and crude oils by distillation. Water co-distills with an immiscible solvent and condenses in a graduated trap. The water settles in the bottom of the trap and is measured.

This method is applicable for the determination of water in crude petroleum oils and crude oils obtained from bituminous minerals (e.g., from shale, calcareous rock, sand). Crude petroleum oils and crude oils obtained from bituminous minerals (e.g., from shale, calcareous rock, sand) are classifiable under the tariff heading of HTSUS 2709 even if they have been subjected to various process such as such decantation, de-salting, dehydration, stabilization in order to normalize the vapor

pressure, or any other minor process, provided it does not change the essential character of the product. Any amount of water present in the crude oil from any of these processes or from any other sources is deductible from the gross standard volume (GSV) of crude petroleum oil to obtain the net standard volume (NSV).

2 REFERENCES

ASTM D 4006

Test Method for Water in Crude Oil by Distillation

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-04

Index

ASTM D 95

Test Method for Water in Petroleum Products and Bituminous Materials By Distillation

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method covers the determination of water in petroleum products, tars, and other bituminous materials by the distillation method. Water co-distills with an immiscible solvent and condenses in a graduated trap. The water settles in the bottom of the trap and is measured.

This method is applicable for the determination of water in crude petroleum oils and crude oils obtained from bituminous minerals (e.g., from shale, calcareous rock, sand). Crude petroleum oils and crude oils obtained from bituminous minerals are classifiable under the tariff heading of HTSUS 2709 even when they have been subjected to various process such as decantation, de-salting, dehydration, stabilization in order to normalize the vapor pressure or any other minor process,

provided it does not change the essential character of the product. Any amount of water present in the crude oil from any of these processes or from any other sources is deductible from the gross standard volume (GSV) of crude petroleum oil to obtain the net standard volume (NSV).

2 REFERENCES

ASTM D 95

Test Method for Water in Petroleum Products and Bituminous Materials by Distillation

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-05

Index

ASTM D 4928 Test Method for Water in Crude Oils by Coulometric Karl Fischer Titration

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

amount of water present in the crude oil from any of these processes or from other sources is deductible from the gross standard volume (GSV) of crude petroleum oil to obtain the net standard volume (NSV).

2 REFERENCES

ASTM D 95

Test Method for Water in Crude Oils by Coulometric Karl Fisher Titration

1 SCOPE AND FIELD OF APPLICATION

This method covers the determination of water in the range of 0.02 to 5 mass % in crude oils by Coulometric Karl Fischer titration. At levels of less than 500 mg/g, the interference of mercaptan and sulfide ($S^{=}$ or H_2S) sulfur is found to be insignificant.

This method is applicable for the determination of water in crude petroleum oils and crude oils. Crude petroleum oils and crude oils obtained from bituminous minerals (e.g., from shale, calcareous rock, sand) are classifiable under the tariff heading of HTSUS 2709 even when they have been subjected to various process such as decantation, de-salting, dehydration, stabilization in order to normalize the vapor pressure or any other minor process, provided it does not change the essential characters of the product. Any

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-06

Index

ASTM D 473 Test Method for Sediment in Crude Oils and Fuel Oils by the Extraction Method

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method covers the determination of sediment in crude oil and fuel oils by extraction with toluene. The extracted residue is calculated in percent unit mass, and reported as "sediment by extraction".

This method is applicable for the determination of the percent sediment in crude oils and fuel oils. The amount of water and sediment (S & W) in crude oil is deductible from the gross standard volume (GSV) to obtain the net observed volume (NSV).

2 REFERENCES

ASTM D 473

Test Method for Sediment in Crude Oils and Fuel Oils by the Extraction Method

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-07

Index

ASTM D 4807

Test Method for Sediment in Crude Oil by Membrane Filtration

2

REFERENCES

ASTM D 4807

Test Method for Sediment in Crude Oil
by Membrane Filtration

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method covers the determination of sediment in crude oils by membrane filtration. The extracted residue is calculated in percent unit mass. This method has been validated for crude oils with sediments up to about 0.15% mass.

This method is applicable for the determination of the amount of sediment in crude petroleum oils and fuel oils. The amount of sediment in crude oil is deductible from the gross standard volume (GSV) to obtain the net standard volume (NSV).

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-08

Index

ASTM D 86 Test Method for Distillation of Petroleum Products

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method covers the distillation of natural gasolines, aviation gasolines, aviation turbine fuels, special boiling point spirits, naphthas, white spirit, kerosines, gas oils, distillates fuel oils, and similar petroleum products, utilizing either manual or automated distillation apparatus. The distillation range of various petroleum distillate products is also determined by this method.

This method is applicable for the determination of percent by volume of aromatic hydrocarbon mixtures in other oils and petroleum distillates which distills at 250°C. The HTSUS specifically lists this method, ASTM D-86, under the subheading of 2707.50 for the determination of the volume quantity (expressed in percent) that distills at 250°C in aromatic hydrocarbon mixtures.

2

REFERENCES

ASTM D 86

Test Method for Distillation of Petroleum Products

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-09

Index

ASTM D 4953 Test Method for Vapor Pressure of Gasoline and Gasoline-Oxygenate Blends (Dry Method)

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

gasolines and gasoline blended fuels based on their vapor pressure.

1 SCOPE AND FIELD OF APPLICATION

This method, a modification of Test Method D-323 [(Reid Method), USCL 27-10] provides two procedures to determine the vapor pressure of gasoline and gasoline-oxygenate blends with vapor pressure range from 35 to 100 kPa (5 to 15 psi). Procedure A utilizes the same apparatus and essentially the same procedure as ASTM D 323 with the exception that the interior surfaces of the liquid and vapor chambers are maintained completely free of water. Procedure B utilizes a semi-automatic apparatus with the liquid and vapor chambers identical in volume to those in Procedure A.

This method is applicable for the determination of the volatility characteristic of automotive spark-ignition engine fuels (per ASTM D-4814, USCL 27-26) such as

2 REFERENCES

ASTM D 4953

Test Method for Vapor Pressure of Gasoline and Gasoline-Oxygenate Blends (Dry Method)

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-10

Index

ASTM D 4953 Test Method for Vapor Pressure of Petroleum Products (Reid Method)

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

determination of the volatility characteristic of automotive spark-ignition engine fuels (per ASTM D-4814, USCL 27-26) such as gasolines, and specific gasoline blended fuels based on their vapor pressure.

1 SCOPE AND FIELD OF APPLICATION

This method covers the determination of the vapor pressure of gasoline, volatile crude oil and other volatile petroleum products. This method consists of four different procedures based on the expected vapor pressure of the petroleum product. Procedure A is applicable to gasoline and other petroleum products with a vapor pressure of less than 180 kPa. Procedure B may also be applicable to these other materials, but only gasoline was included in the interlaboratory test program to determine the precision of this test method. Neither procedure is applicable to liquefied petroleum gases or fuels containing oxygenated compounds other than methyl t-butyl ether (MTBE). Procedure C is for materials with a vapor pressure of greater than 180 kPa and Procedure D is for aviation gasoline with a vapor pressure of approximately 50 kPa.

This method is applicable for the

2 REFERENCES

ASTM D 4953

Test Method for Vapor Pressure of Petroleum Products (Reid Method)

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-11

Index

ASTM D 445

Test Method for Kinematic Viscosity of Transparent and Opaque Liquids (the Calculation of Dynamic Velocity)

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method involves the determination of the kinematic viscosity, ν , of liquid petroleum products, both transparent and opaque, by measuring the time for a volume of liquid to flow under gravity through a calibrated glass capillary viscometer. The dynamic viscosity, η , can be obtained by multiplying the measured kinematic viscosity by the density, ρ , of the liquid.

This method is applicable for the determination of the kinematic viscosity of transparent and opaque liquids such as various petroleum distillate products and fuel oils. Various petroleum distillate products and fuel oils (including blended fuel oils) are characterized by their

viscosity. Petroleum distillates and residual fuel oils are classifiable in the HTSUS according to their viscosity expressed in Saybolt Universal Seconds at 37.8 °C. The viscosity of a fuel oil also determines its use.

2 REFERENCES

ASTM D 445

Test Method for Kinematic Viscosity of Transparent and Opaque Liquids (the Calculation of Dynamic Velocity)

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-12

Index

ASTM D 88 Test Method for Saybolt Viscosity

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method covers the empirical procedures for determining the Saybolt Universal or Saybolt Furol viscosity of petroleum products at specified temperatures between 21 and 99°C (70 and 210°C).

This method is applicable for the determination of Saybolt Universal or Saybolt Furol viscosities of petroleum products and fuel oils. The Saybolt Furol is recommended for fuel oils having Saybolt Universal viscosities greater than 1000s. Various petroleum distillate products and fuel oils (including blended fuel oils) are characterized by their viscosity. Petroleum distillates and residual fuel oils are classifiable in the HTSUS according to their viscosity expressed in Saybolt Universal at 37.8 °C. The viscosity of fuel oils also determines its use.

2

REFERENCES

ASTM D 88

Test Method for Saybolt Viscosity

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-13

Index

ASTM D 4294 **Test Method for Sulfur in Petroleum Products by** **Energy-Dispersive X-Ray Fluorescence Spectroscopy**

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This test method covers the measurement of sulfur in hydrocarbons from petroleum commodities. It covers a range of from 0.05 to 5% by mass.

2 REFERENCES

ASTM D 4294

Test Method for Sulfur in Petroleum Products by Energy-Dispersive X-Ray Fluorescence Spectroscopy

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-14

Index

ASTM D 2622 **Test Method for Sulfur in Petroleum Products** **(X-Ray Spectrographic Methods)**

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method covers the determination of the total sulfur in liquid petroleum products or petroleum products that can be liquified with slight heating. This method should be used under the following set of conditions: petroleum crude oil, paraffinic sample, and sulfur concentrations not to exceed 0.0010 % by mass.

2 REFERENCES

ASTM D 2622

Test Method for Sulfur in Petroleum Products (X-Ray Spectrographic Methods)

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-15

Index

ASTM D 3437

Practice for Sampling and Handling Liquid Cyclic Products

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method covers the sampling and handling of several of the cyclical organic commodities. Most of these commodities have a safety and/or a fire hazard associated with them. This method discusses some of the hazards that have to be addressed in unloading and sampling these commodities contained within drums, tank trucks, and rail cars.

2 REFERENCES

ASTM D 3437

Practice for Sampling and Handling
Liquid Cyclic Products

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-16

Index

ASTM E 300 Practice for Sampling Industrial Chemicals

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method covers good industrial sampling practices in order to meet the statistical requirements of a representative sample. It discusses the equipment and techniques required to obtain a good sample for the following general types of commodities: liquids, solids, and slurries.

2 REFERENCES

ASTM E 300
Practice for Sampling Industrial Chemicals

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-17

Index

ASTM D 3438

Practice for Sampling and Handling Naphthalene, Maleic Anhydride, and Phthalic Anhydride

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method covers the sampling and handling of naphthalene, maleic anhydride, and phthalic anhydride in the various forms of solid and molten states. There are serious health, safety, fire, and explosion hazards associated with the sampling and handling of these substances.

2 REFERENCES

ASTM D 3438

Practice for the Sampling and Handling
Naphthalene, Maleic Anhydride, and
Phthalic Anhydride

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-18

Index

ASTM D 3852 **Practice for Sampling and Handling Phenol** **and Cresylic Acid**

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method covers the sampling and handling of phenol, cresylic acid, and their sodium salts. These commodities have serious health, safety, and fire hazards that must be addressed. This procedure covers the appropriate techniques that must be followed in dealing with these substances.

2 REFERENCES

ASTM D 3852

Practice for the Sampling and Handling Phenol and Cresylic Acid

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-19

Index

ASTM D 3439

Test Methods for Assay of Alkaline Cresylate Solutions from Petroleum Sources

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method covers the neutralization, separation, and identification of the various constituents of the sodium cresylate salts. These commodities are normally produced as a waste by-product from certain petroleum refinery waste streams that are treated with caustic. This procedure analyzes the water, sulfur, neutral oil, and a certain distillate fraction of the waste commodity. This assay will allow the analyst to define such a commodity for the tariff.

2 REFERENCES

ASTM D 3439

Test Methods for Assay of Alkaline
Cresylate Solutions from Petroleum
Sources

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-20

Index

ASTM D 4057 **Practice for Manual Sampling of Petroleum** **and Petroleum Products**

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method covers procedures for obtaining representative samples of uniform petroleum liquid and solid products. All of the liquid petroleum commodities are covered with this method except the transformer and hydraulic oils. Greases and asphalt solid petroleum commodities are also covered with this method. This method also covers the industrial aromatic hydrocarbons, naphthas, and gasolines. The following techniques are covered: running sampling; all levels sampling; continuous sampling; and thief sampling.

2 REFERENCES

ASTM D 4057

Practice for Manual Sampling of
Petroleum and Petroleum Products

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-21

Index

ASTM D 4177 **Practice for the Automatic Sampling of Petroleum** **and Petroleum Products**

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This procedure covers all of the engineering specifications required to achieve a representative sample by using an automatic mechanical means. The specific details of the piping requirements are discussed and subsequent calibration programs are covered. All of the necessary calculations are covered in relation to the equipment including the flowmeter that sets the pace of the whole automatic sampling process.

2 REFERENCES

ASTM D 4177

Practice for the Automatic Sampling
of Petroleum and Petroleum
Products

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-22

Index

ASTM D 396 Specification for Fuel Oils

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method lists all of the physical and chemical specifications of the various grades of fuel oils. An analyst should compare the physical and chemical test results of the petroleum commodity in question to those listed in this method in order to classify the commodity as a specific grade of fuel oil.

2 REFERENCES

ASTM D 396
Specification for Fuel Oils

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-23

Index

ASTM D 975 Specification for Diesel Fuel Oils

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method lists all of the physical and chemical specifications of diesel fuel oils. It should be used to help define a petroleum commodity as a diesel fuel by comparing its physical and chemical properties to those listed in this method.

2 REFERENCES

ASTM D 975

Specification for Diesel Fuel Oils

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-24

Index

ASTM D 2069 Specification for Marine Fuels

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method lists the chemical and physical properties of the various grades of marine fuel oils. The analyst should compare the properties of the petroleum commodity in question with the properties listed in this method in order to classify the commodity.

2 REFERENCES

ASTM D 2069
Specification for Marine Fuels

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-25

Index

ASTM D 2880 Specification for Gas Turbine Fuel Oils

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

- 1.1 This specification covers the selection of fuels for gas turbines, excepting gas turbines used in aircraft.
- 1.2 The specification sets forth the properties of fuels at the time of exportation from the source country to the United States of America, as it pertains to heading 2710 of the Harmonized Tariff Schedule of the United States (HTSUS).

2 REFERENCES

ASTM D 2880

Specification for Gas Turbine Fuel Oils

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-26

Index

ASTM D 4814

Specification for Automotive Spark-Ignition Engine Fuel

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

- 1.1 This specification guides in establishing requirements of automotive fuels for ground vehicles equipped with spark-engines.
- 1.2 The specification sets forth the properties of fuels at the time of exportation from source country to the United States of America as it pertains to heading 2710 of the Harmonized Tariff Schedule of the United States (HTSUS).
- 1.3 The spark-ignition engine fuels covered in this specification are gasoline and its blends with oxygenates such as alcohols and ethers.
- 1.4 This specification does not apply to fuels that contain an oxygenate as primary component, such as Fuel Methanol (M85).

1.5 The concentrations and the types of oxygenates are not specifically limited in this specification.

1.6 This specification describes characteristics of automotive fuels for use over a wide range of operating conditions. The specification neither necessarily includes all types of fuels that are satisfactory for automotive vehicles, nor necessarily excludes fuels that can perform unsatisfactorily under certain operating conditions or in certain equipment.

1.7 This specification represents a description of automotive fuels as of date of publication. The specification is under continuous review, which can result in revisions based on changes in fuel, automotive requirements, or test methods, or combination thereof. Therefore, the latest edition of the specification must be referred to at all times.

2 REFERENCES

ASTM D 4814

Specification for Automotive Spark-Ignition Engine Fuel

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-27

Index

ASTM D 1655 Specification for Aviation Turbine Fuels

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

than turbine engines which are specifically designed and certified for this fuel.

2

REFERENCES

ASTM D 1655

Specification for Aviation Turbine Fuels

1 SCOPE AND FIELD OF APPLICATION

- 1.1 This specification sets forth the properties of aviation turbine fuels at the time of exportation from the source country to the United States of America as it pertains to heading 2710 of the Harmonized Tariff Schedule of the United States (HTSUS).
- 1.2 The specification defines specific types of aviation turbine fuels.
- 1.3 The specification does not include all fuels satisfactory for aviation turbine engines. Certain equipment or conditions of use may permit a wider, or require a narrower, range of characteristics than is shown by this specification.
- 1.4 Aviation turbine fuels defined by this specification may be used in other

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-28

Index

ASTM D 910 Specification for Aviation Gasolines

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

2 REFERENCES

ASTM D 910

Specification for Aviation Gasolines

1 SCOPE AND FIELD OF APPLICATION

- 1.1 This specification sets forth the properties of aviation gasoline fuels at the time of exportation from the source country to the United States of America as it pertains to heading 2710 of the Harmonized Tariff Schedule of the United States (HTSUS).
- 1.2 This specification defines specific types of aviation gasolines.
- 1.3 The specification does not include all gasoline satisfactory for reciprocating aviation engines. Certain equipment or conditions of use may permit a wider, or require a narrower, range of characteristics than is shown by this specification.

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-29

Index

ASTM D 3699 Specification for Kerosine

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

pertains to heading 2710 of the Harmonized Tariff Schedule of the United States(HTSUS).

2

REFERENCES

ASTM D 3699
Specification for Kerosine

1 SCOPE AND FIELD OF APPLICATION

1 SCOPE AND FIELD OF APPLICATION

1.1 This specification covers two grades of kerosine suitable for use in critical kerosine burner applications:

1.1.1 No. 1-K--A special low sulfur grade kerosine suitable for use in non-flue-connected kerosine burner appliances, and for use in wick-fed illuminating lamps;

1.1.2 No. 2-K--A regular grade kerosine suitable for use in flue-connected burner appliances and for use in wick-fed illuminating lamps.

1.2 The specification sets forth the properties of kerosine at the time of exportation from the source country to the United States of America as it

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-30

Index

ASTM D 235 Specification for Mineral Spirits (Petroleum Spirit) (Hydrocarbon Dry Cleaning Solvent)

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

2 REFERENCES

ASTM D 235

Specification for Mineral Spirits
(Petroleum Spirits)(Hydrocarbon Dry
Cleaning Solvent)

1 SCOPE AND FIELD OF APPLICATION

- 1.1 This specification covers four types of hydrocarbon solvents, normally petroleum distillates, used primarily in coatings and dry-cleaning industries. "Mineral Spirits" is the most common name for these solvents. They are also called "Stoddard Solvents" when used for dry-cleaning.
- 1.2 The specification sets forth the properties of hydrocarbon solvents at the time of exportation from the source country to the United States of America, as it pertains to heading 2710 of the Harmonized Tariff Schedule of the United States (HTSUS).

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-31

Index

ASTM D 3735 Specification for VM&P Naphthas

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

2

REFERENCES

ASTM D 3735
Specification for VM&P Naphthas

1 SCOPE AND FIELD OF APPLICATION

1.1 This specification covers three types of moderately volatile hydrocarbon solvents, mainly aliphatic in composition and normally petroleum distillates. These solvents are used primarily by the coating industry and are commonly referred to as VM&P naphthas.

1.2 The specification sets forth the properties of moderately volatile hydrocarbon solvents at the time of exportation from the source country to the United States of America, as it pertains to heading 2710 of the Harmonized Tariff Schedule of the United States (HTSUS).

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-32

Index

ASTM D 938 Test Method for Congealing Point of Petroleum Waxes Including Petrolatum

2 REFERENCES

ASTM D 938

Test Method for Congealing Point of
Petroleum Waxes including Petrolatum

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

- 1.1 This test method covers the determination of the congealing point of petroleum waxes, including petrolatum.
- 1.2 The values stated in inch-pound units are to be regarded as the standard.
- 1.3 This test method covers the petroleum waxes, including petrolatum imported under heading 2712 of the Harmonized Tariff Schedule of the United States (HTSUS).

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-33

Index

ASTM D 5 Test Method for Penetration of Bituminous Materials

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

- 1.1 This method covers determination of the penetration of semi-solid and solid bituminous material.
- 1.2 This test method cover bituminous material imported under headings 2713, 2714, and 2715 of the Harmonized Tariff Schedule of the United States (HTSUS).

2 REFERENCES

ASTM D 5

Test Method for Penetration of Bituminous Materials

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-34

Index

ASTM D 217 Test Method for Cone Penetration of Lubricating Grease

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

1.1 These test methods cover four procedures for measuring the consistency of lubricating greases by the penetration of a cone of specified dimensions, mass, and finish. The penetration is measured in tenths of a millimeter.

1.1.1 The procedures for unworked, worked, and prolonged worked penetration are applicable to greases having penetrations between 85 and 475, that is, to greases with consistency numbers between (National Lubricating Grease Institute) NLGI 6 and NLGI 000.

1.1.2 The block penetration procedure is applicable to greases that are sufficiently hard to hold their shape. Such greases usually have

penetration below eighty-five tenths of a millimeter.

1.2 None of the four procedures is considered suitable for measurement of petrolatum by penetration.

1.3 These test methods cover the lubricating greases imported under heading 2710 of the Harmonized Tariff Schedule of the United States (HTSUS).

2 REFERENCES

ASTM D 217

Test Method for Cone Penetration of Lubricating Grease

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-35

Index

ASTM D 937 Test Method for Cone Penetration of Petroleum

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

- 1.1 This test method covers measuring with a penetrometer the penetration of petrolatum as an empirical measure of consistency.
- 1.2 SI units are to be regarded as standard to state the values.
- 1.3 This test method covers the petrolatum imported under heading 2712 of the Harmonized Tariff Schedule of The United States (HTSUS).

2 REFERENCES

ASTM D 937
Test Method for Cone Penetration of Petroleum

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-36

Index

ASTM D 1265 Practice for Sampling Liquid Petroleum (LP) Gases (Manual Method)

Harmonized Tariff schedule of the
United States (HTSUS).

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

2

REFERENCES

ASTM D 1265
Practice for Sampling Liquefied
Petroleum (LP) Gases (Manual
Method)

1 SCOPE AND FIELD OF APPLICATION

- 1.1 This practice covers the procedure for obtaining representative samples of liquefied petroleum gases such as propane, butane, or mixtures thereof, in containers other than those used in laboratory testing apparatus. These procedures are considered adequate for obtaining representative samples for all routine tests for LP gases required by Specification D 1835 except analysis by test method D-2163. They are not intended for obtaining samples to be used for compositional analysis. A sample procedure that avoids changes in composition must be used for compositional analysis.
- 1.2 This sampling procedure covers the liquefied petroleum (LP) gases imported under heading 2711 of the

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-37

Index

ASTM E 137

Practice for Evaluation of Mass Spectrometers for Quantitative Analysis from a Batch Inlet

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

The title of this method is also the scope of this method. It is useful for determining the suitability of a particular mass spectrometer for the purpose of analyzing organic compounds quantitatively from a batch inlet. This method was discontinued by ASTM in 1992.

2 REFERENCES

ASTM E 137

Practice for Evaluation of Mass
Spectrometers for Quantitative
Analysis from a Batch Inlet

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-38

Index

ASTM D 2650 Test Method for Chemical Composition of Gases by Mass Spectrometry

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

The scope of this method is magnetic sector mass spectrometric quantitative analysis down to the lower limit of 0.1 mole percent of the following gases: hydrocarbons with six or fewer carbon atoms per molecule; carbon monoxide; carbon dioxide; mercaptans with one or two carbon atoms per molecule; hydrogen sulfide; air; nitrogen; oxygen; argon; and hydrogen.

This method is applicable to the quantitative analysis of light hydrocarbon gasses as listed in Chapter 27.

2 REFERENCES

ASTM D 2650

Test Method for Chemical
Composition of Gases by Mass
Spectrometry

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-39

Index

ASTM D 721 Test Method for Oil Content of Petroleum Waxes

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

The scope of this method covers the determination of the oil content of petroleum wax where the wax has a congealing point of less than 30 degrees C and an oil content of less than 15 percent. This method is applicable to the determination of the oil content of paraffin wax in Chapter 27.

2 REFERENCES

ASTM D 721

Test Method for Oil Content of Petroleum Waxes

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-40

Index

ASTM D 140 Practice for Sampling Bituminous Materials

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

The scope of this method covers the sampling of bituminous materials at points of manufacture, storage, and delivery. It is applicable to the sampling of such materials as listed in Chapter 27 for analysis.

2 REFERENCES

ASTM D 140
Test Method for Sampling
Bituminous Materials

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-41

Index

ASTM D 977 Specifications for Emulsified Asphalts

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method specifies twelve grades of emulsified asphalt for use in pavement construction. It is applicable to the classification of petroleum asphalt in Chapter 27.

2 REFERENCES

ASTM D 977

Specification for Emulsified Asphalt

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-42

Index

ASTM D 244 Test Methods for Emulsified Asphalts

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method covers standard test methods for the examination of asphalt emulsions. It is applicable to the analysis and classification of petroleum asphalt in Chapter 27.

2 REFERENCES

ASTM D 244

Test Methods for Emulsified Asphalts

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-43

Index

ASTM D 2026 Specifications for Cutback Asphalt (Slow Curing Type)

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method describes the specifications for cutback asphalt. It is applicable to the classification of asphalt in Chapter 27.

2 REFERENCES

ASTM D 2026
Specifications for Cutback Asphalt
(Slow Curing Type)

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-44

Index

ASTM D 2027 Specifications for Cutback Asphalt (Medium Curing Type)

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method describes the specifications for cutback asphalt, medium curing type. It is applicable to the classification of asphalt in Chapter 27.

2 REFERENCES

ASTM D 2027

Specifications for Cutback Asphalt
(Medium Curing Type)

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-45

Index

ASTM D 2028 Specifications for Cutback Asphalt (Rapid Curing Type)

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

1 SCOPE AND FIELD OF APPLICATION

This method describes the specifications for cutback asphalt, rapid curing type. It is applicable to the classification of asphalt in Chapter 27.

2 REFERENCES

ASTM D 2028

Specifications for Cutback Asphalt
(Rapid Curing Type)

U.S. CUSTOMS LABORATORY METHODS

USCL METHOD 27-47

INDEX

Guidelines For Country-of-Origin Determinations Of Distillate Petroleum Products From Iraq

SAFETY PRECAUTIONS

This method does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this method to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.

0 INTRODUCTION

There has been strong evidence for the organic origin of petroleum since 1936 when Treibs demonstrated a link between chlorophyll-a in living photosynthetic organisms and porphyrins in petroleum (9.1). His work marked the beginning of modern organic geochemistry by his demonstration of the biological origin of a specific compound found in crude oil. Such compounds are known as biomarkers. Formally, we define biomarkers as compounds found in petroleum that are derived from previously living organisms.

Biomarkers found in petroleum are useful for determining the origin of petroleum because their relative concentrations vary from oil field to oil field. This variation is due to differences in source organic input material, depositional conditions, age of the oil, and integrated oil temperature over geologic time (9.2, 9.3). The petroleum geochemistry and

analytical chemistry of pristane, phytane, and heavier molecular weight biomarkers have been extensively discussed and developed in the literature (9.4-9.7).

Additionally, compound specific isotope ratio mass spectrometry has recently been used to extend our geochemical understanding of petroleum development to include low molecular weight biomarkers in the n-C4 through n-C20 region (9.8-9.10). Moreover, new compounds continue to be identified, described in the literature, and established as biomarkers useful for oil source correlations (9.11,9.12).

The cited literature and references therein have clearly established that biomarkers extend through the entire molecular weight range of petroleum. Therefore, for the purpose of determining the origin of a petroleum sample, it is only necessary that the compounds used for comparison purposes vary in their relative concentration with respect to each other from oil field to oil field.

1 SCOPE AND FIELD OF APPLICATION

This method describes the determination of the origin of a petroleum sample by the analysis of an entire high resolution capillary gas chromatogram from the instant sample and all consulted reference samples. Also discussed are a series of biomarker and other low molecular weight compounds

whose concentrations vary widely among various oil fields.

In this regard, a preliminary screening of any complex petroleum mixture can be performed by the profile analysis of a wide variety of compounds, while a detailed analysis of specific regions of the chromatograms is necessary to distinguish between two very similar, yet different, petroleum oils. The specific problem of the determination of the origin of a petroleum sample via its profile is but one representative of the general class of problems known as Profiling Complex Mixtures (9.13). This profiling is rooted in mathematics, whereby, the fundamental problem is to determine if two objects are the same, a very difficult task when two objects are distinct, yet very similar (9.14).

The comparison of an instant petroleum sample to one or more reference petroleum samples is a mathematical problem in the specialized subject area of pattern recognition. Methods by which pattern recognition occur range from a visual comparison where the mathematics are performed in some unknown manner by the human brain to a numerical comparison where the mathematics are performed by a computer using a known and well described set of data in conjunction with a software program, compiler, and operating system with known and available source code. This method describes a primary method for visual pattern recognition and a supplementary method for determining the relative mathematical similarity of a sample chromatogram to the members of a set of reference chromatograms.

2 REFERENCES

"Country-of-Origin Determinations of Distillate Petroleum Products From Iraq"
Neal D. Byington and Larry D. Fluty
Customs Laboratory Bulletin
(submitted)

3 REAGENTS AND APPARATUS

- 3.1 Hewlett/Packard Model 5890 Series II Plus capillary gas chromatograph with a split/splitless injector, flame ionization detector, liquid carbon dioxide sub-ambient cooling oven attachment, autosampler control module, and electronic pressure control.
- 3.2 Hewlett/Packard Model 7673A autosampler fitted with a 10 μ L syringe
- 3.3 Hewlett/Packard Chem Station and software (PC)
- 3.4 Gas Chromatograph operating conditions
 - 3.4.1 Split/splitless injector with a cup injector liner
 - 3.4.2 J&W DB-1, 60 meter, capillary column, part number 122-1063. This non-polar column has a one micron film thickness and an internal diameter of 0.25 mm.
 - 3.4.3 Compressed helium carrier gas with a regulator for the capillary column.
 - 3.4.4 Compressed air with a regulator for the FID detector.
 - 3.4.5 Compressed hydrogen with a regulator for the FID detector.
 - 3.4.6 Compressed carbon dioxide with a liquid dip tube feeder to provide liquid carbon dioxide cooling to the gas chromatograph oven.
 - 3.4.7 Supelco High Capacity Gas Purifier
 - 3.4.8 Supelco Thermogreen LB-2 septum.

- 3.5** Eppendorf pipets:
a) 100 μ L pipet
b) variable 100-1000 μ L pipet
- 3.6** Vortex Mixer
- 3.7** Cyclohexane, ACS reagent grade
- 3.8** Reference samples:
- 3.8.1** Gasoline
- 3.8.2** Kerosine
- 3.8.3** Crude oil
- 3.8.4** Distillate fuel oil
- 3.8.5** Crude oil samples from oil fields of relevance to the instant analytical sample

4 SAMPLE PREPARATION

- 4.1** To prepare a sample of distillate petroleum for the gas chromatograph, 100 μ L of distillate petroleum and 900 μ L of cyclohexane are measured into a GC vial and capped.
- 4.2** Vortex the mixture for 15 seconds.

5 EXPERIMENTAL PROCEDURE

- 5.1** The autosampler is loaded to run a set of samples such that each of the first two vials, the last vial, and one vial between each sample vial is a blank vial of cyclohexane. This provides significant evidence that the gas chromatograph is operating properly both before and after the analysis of any specific sample.
- 5.2** A 1.0 μ L sample of the mixture is injected into the gas chromatograph via an autosampler using a 10 μ L syringe.

5.3 Gas Chromatograph run conditions

- 5.3.1** The helium column carrier gas is under electronic pressure control with a column flow rate set at 1.5 mL/min \pm 0.1 mL/min at 30 degrees C. The helium carrier gas is purified through an electrically heated Supelco High Capacity Gas Purifier
- 5.3.2** Split/splitless injector (cup injector liner packed with 10% OV-1 on Chromosorb-W) is used in the split mode at a split vent volume of 140 mL/min \pm 2.0 mL/min
- 5.3.3** The temperature of the injection port is isothermally maintained at 275 EC.
- 5.3.4** The oven temperature controller is set to hold the oven temperature for 5 minutes at 30 EC via liquid carbon dioxide sub-ambient cooling of the oven and then to ramp the oven at 5 EC/min to 275 EC and hold it at that temperature for
- a) 6 minutes for gasoline range material,
 - b) 40 minutes for mid-range distillate material,
 - c) 90 minutes for crude oil.
- 5.3.5** The temperature of the detector is isothermally maintained at 275 EC.

6 PRECISION

- 6.1** The resolution of the column is considered to be adequate when the system provides baseline resolution of the following compounds using the conditions described in the experimental procedure.
- 6.1.1** For gasoline and kerosine distillation range materials, trans-2-butene and cis-2-butene

- 6.1.2** For crude oil and distillate fuel oil materials, n-C17/pristane and n-C18/phytane peak pairs.

7 RESULTS

- 7.1** Figures I through IV are the high resolution capillary gas chromatograms of the profile and three key comparison sections of a distillate fuel oil obtained from Basrah Light crude oil from Iraq.

- 7.1.1** Figure I, Distillate Fuel Oil Obtained From Basrah Light Crude Oil, is the entire profile chromatogram of the sample.

- 7.1.2** Figure II, Distillate Fuel Oil Obtained From Basrah Light Crude Oil, is the partial chromatogram of the sample in the n-C8 through n-C9 hydrocarbon range.

- 7.1.3** Figure III, Distillate Fuel Oil Obtained From Basrah Light Crude Oil, is the partial chromatogram of the sample in the n-C9 through n-C11 hydrocarbon range.

- 7.1.4** Figure IV, Distillate Fuel Oil Obtained From Basrah Light Crude Oil, is the partial chromatogram of the sample in the n-C16 through phytane hydrocarbon range.

- 7.2** Figures V through VIII are the high resolution capillary gas chromatograms of the profile and three key comparison sections of Iranian Heavy crude oil from Iran.

- 7.2.1** Figure V, Iranian Heavy Crude Oil, is the entire profile chromatogram of the sample.

- 7.2.2** Figure VI, Iranian Heavy Crude Oil, is the partial chromatogram of the sample in the n-C8 through n-C9 hydrocarbon range.

- 7.2.3** Figure VII, Iranian Heavy Crude Oil, is the partial chromatogram of the sample in the n-C9 through n-C11 hydrocarbon range.

- 7.2.4** Figure VIII, Iranian Heavy Crude Oil, is the partial chromatogram of the sample in the n-C16 through phytane hydrocarbon range.

8 GUIDELINES FOR COUNTRY-OF-ORIGIN DETERMINATIONS

- 8.1** Introduction

- 8.1.1** The country-of-origin of a petroleum sample is determined by a chemist following an examination of all available data, including a detailed comparison of the entire gas chromatogram for the sample and all consulted reference samples with particular attention to selected compounds whose relative concentrations are very sensitive to origin-dependent factors.

The selection of how many and which reference samples and specific compounds within those samples to use for detailed origin dependent comparison purposes may change as examination of an instant sample proceeds. The detailed comparison of an instant sample with selected reference samples can be performed by any of a variety of individual techniques or a combination of techniques which range from visual to mathematical comparisons of the relevant data.

Supplemental analytical methodology and other data of any type and from any source may be used to provide additional data to assist in the determination of the country-of-origin of an instant sample. The scope of this section encompasses two sets of guidelines, one visual and the other mathematical, for the

determination of the country-of-origin of distillate petroleum products from Iraq.

8.1.2 The relative ratios of the selected origin-dependent gas chromatographic peaks must vary between oils of different origin and remain relatively constant from tanker to tanker for oils of the same origin.

8.1.3 Each peak in a gas chromatogram of a complex mixture such as a crude oil or any distillate fraction probably consists of more than one organic compound. It is not necessary to know the identity of the major compound in each peak that is used for comparison purposes.

8.2 Visual Comparison Guidelines

8.2.1 In all cases, chromatographic data from an instant sample are visually compared with similar data from selected reference samples.

8.2.1.1 In all cases, raw chromatographic data obtained by the experimental procedure as described in section 5, using the sample preparation as described in section 4, and using the equipment as described in section 3, are processed into the formats of Figures I through IV and analyzed as described in sections 8.2.2 through 8.2.5.

8.2.2 Figure I provides the entire chromatogram which clearly illustrates the very general chromatographic profile features that are common to this distillate product from Iraq.

8.2.2.1 Of particular note in Figure I is the very wide asymmetrical distillate range from n-C7

through n-C26 that is centered in the n-C13 to n-C14 region.

8.2.2.2 This fuel oil contains distillate material from the top of the naphtha region in the gasoline range, through the number one fuel oil kerosine range, through the number two fuel oil/diesel fuel range, and up into the bottom of the number four fuel oil range. It is a straight-run distillate fuel oil from a distillation tower that is maximized to produce distillate fuel oils suitable for use in either diesel engines or heating stoves.

8.2.3 Figure II provides an expansion of the entire chromatogram covering the n-C8 to the n-C9 range.

8.2.3.1 The light hydrocarbons between these two n-alkanes have very distinctive relative ratios which prominently reflect origin differences among many crude oils, particularly those very similar oils on the Western side of the Arabian Gulf.

8.2.3.2 The peaks at retention indexes of 832, identified in the literature as n-propylcyclopentane, and 844, similarly identified in the literature as 1,1,3-trimethylcyclohexane, are very significant(9.10).

8.2.3.3 It has been observed that these compounds have consistently and uniquely remained approximately equal in intensity for Basrah Light derived fuel oils.

8.2.4 Figure III provides an expansion of the entire chromatogram covering

the n-C9 to the n-C11 range.

8.2.4.1 The light hydrocarbons between these two n-alkanes have a general pattern that is very sensitive to origin differences.

8.2.4.2 In the n-C9 to n-C10 region, there are two sets of unidentified doublet peaks that are of particular interest.

8.2.4.2.1 The leftmost of the first set is at an uncorrected retention index of 964 while the leftmost of the second set is at an uncorrected retention index of 973.

8.2.4.2.2 For Basrah Light crude oil derived distillate fuel oils, the right member of each set is of a lower peak height than the leftmost member of each set.

8.2.4.3 In the n-C10 to n-C11 region, there are two sets of unidentified triplets that are of particular interest.

8.2.4.3.1 The rightmost member of the first set is at an uncorrected retention index of 1026, and similarly, the rightmost member of the second set is at 1066.

8.2.4.3.2 For Basrah Light crude oil derived distillate fuel oils, the rightmost members of each set are higher than those to the left.

8.2.5 Figure IV provides an expansion of the entire chromatogram covering the n-C16 to the phytane region.

8.2.5.1 Using uncorrected retention indexes, of particular interest is the relationship between the peak for phytane at 1816, a peak that is predominately pristane at 1712, and two unidentified peaks at 1674 and 1654.

8.2.5.1.2 For oils obtained from Basrah Light crude oil and some other Northwest Arabian Gulf crude oils, a nearly straight line can be drawn across the top of the peaks at uncorrected retention indexes of 1816, 1712, and 1674 which will intersect the peak at 1654 at one half to three quarters of its' height.

8.2.5.1.3 The very low pristane and phytane peak heights relative to the adjacent n-alkanes is indicative of a very old organic source input material and characteristic of many oils in the Western Arabian Gulf, and this, among many other differences, distinguishes them from the Iranian oils.

8.3 Mathematical Comparison Guidelines

8.3.1 Visual pattern recognition may be assisted by mathematical techniques. A purely mathematical

	analysis is available through the use of the PASCAL program, PASCAL Pattern Similarity Program (PPSP). A detailed description of this program including full source code is provided in Annex I . This program, PPSP, provides a numerical measure of the similarity between sample and reference chromatograms. (9.13, 9.15-9.18).	8.3.2.4	Develop the reference data set file as described in Annex I, 1.1, and 1.4 .
8.3.1.1	In all cases where mathematical techniques are used, chromatographic data from an instant sample and all selected reference samples are visually compared before and after any mathematical comparisons. The conclusions from both the visual and the mathematical techniques are examined by the chemist prior to determining an origin.	8.3.2.5	Full source code for the program is provided in Annex 1.8 . Further refinement may be obtained by modifying the source code to permit the program to use different Minkowski Distances. A listing of alternate Minkowski Distances and why they may be useful is provided in Annex 1.5 . A list of the procedures whose source code must be modified to enable alternate Minkowski Distances to be utilized is provided in Annex 1.6 . A list of each procedure in the PPSP is provided in Annex 1.2 .
8.3.2	The program, PPSP, will accept chromatographic data in the form of either peak heights or peak areas. Visual comparisons are more easily interpreted if peak height data are used in the mathematical program, but either is acceptable.	8.3.2.6	Compile and run PPSP with the developed sample and reference data files according to the directions in Annex 1.1 .
8.3.2.1	Select at least four peaks from the chromatogram whose height or area varies with the origin of the petroleum sample.	8.3.2.7	The results file from PPSP will provide a mathematical metric distance between the data points for the chromatographs from the instant sample to each reference sample. The mathematical distances between chromatographs are sorted by numerical distance and are computed for two different metrics.
8.3.2.2	Select reference samples from suspect origin oils and other oils similar to the instant sample oil.	8.3.2.8	The reference samples with the smallest Minkowski metric distances are considered to be more similar to the instant sample than those whose distances are larger.
8.3.2.3	Develop the sample data set file as described in Annex I, 1.1, and 1.3 .		

9 BIBLIOGRAPHY

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1988.

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Annex 1 PASCAL Pattern Similarity Program (PPSP)

Annex 1.1 Directions on How to Use the PPSP

Annex 1.2 Listing and Description of Each Procedure in the PPSP

Annex 1.3 Example of a Sample Data File

Annex 1.4 Example of a Reference Data File

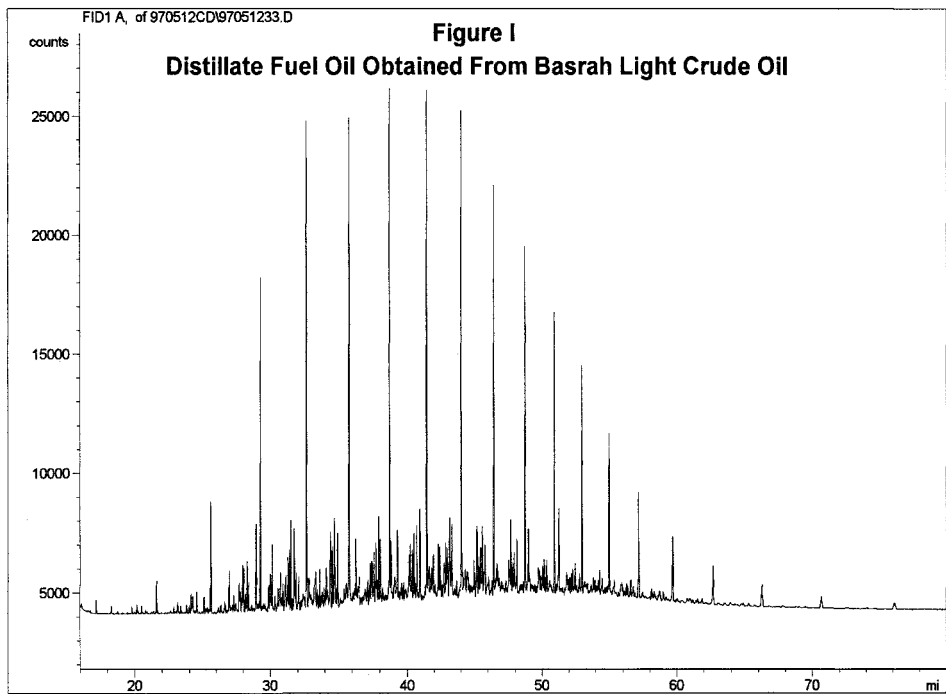
Annex 1.5 Example of a Sample Results File

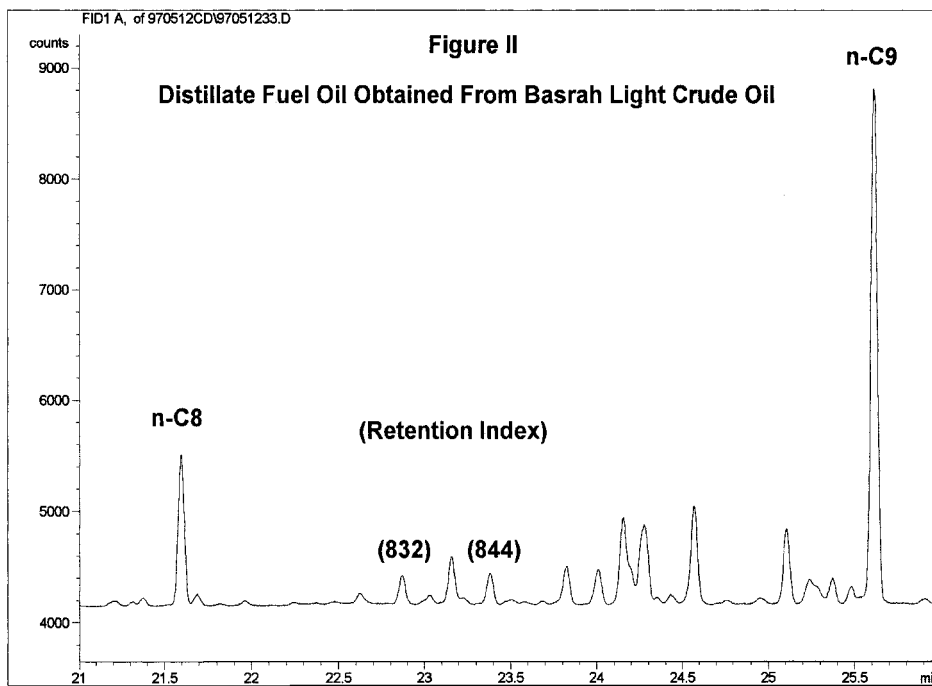
Annex 1.6 Discussion and List of Alternate Minkowski Distance Parameters

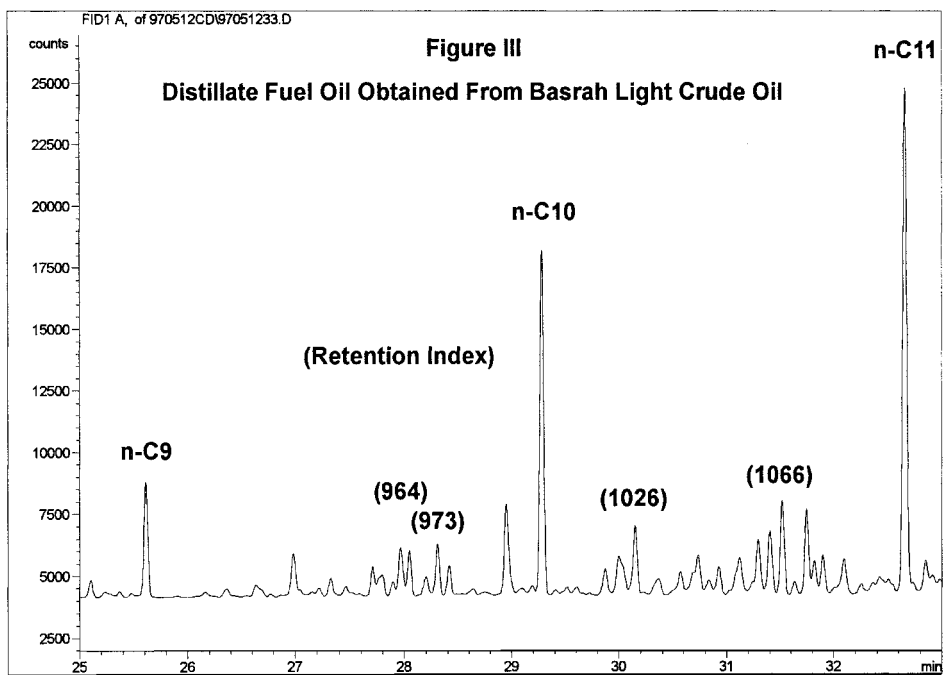
Annex 1.7 List of Procedures Whose Source Code Must Be Modified to Enable PPSP to Use Different Minkowski Distance Parameters

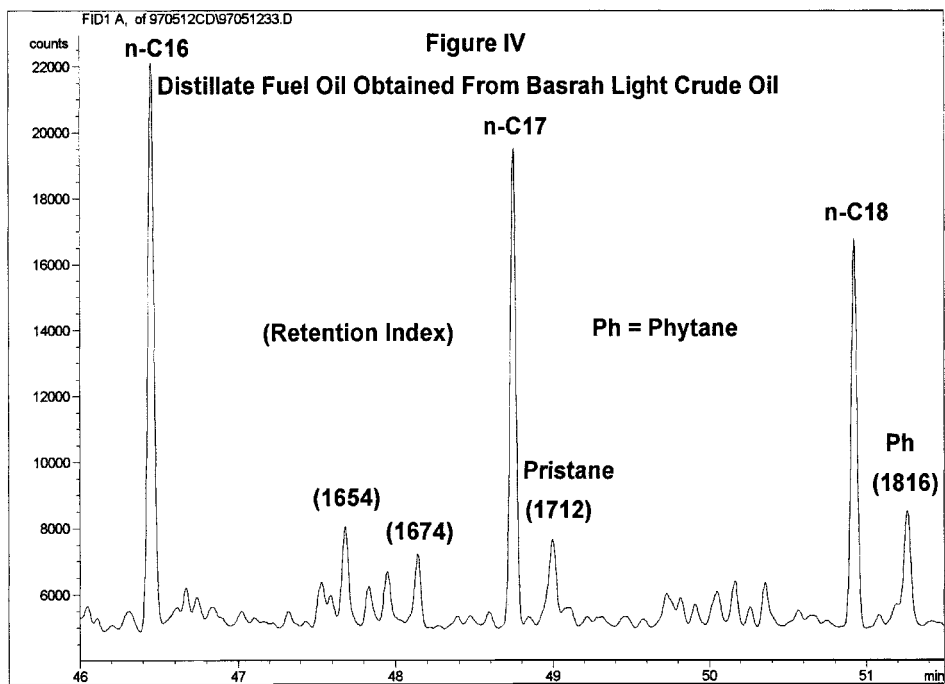
Annex 1.8 Pascal Compiler Requirements

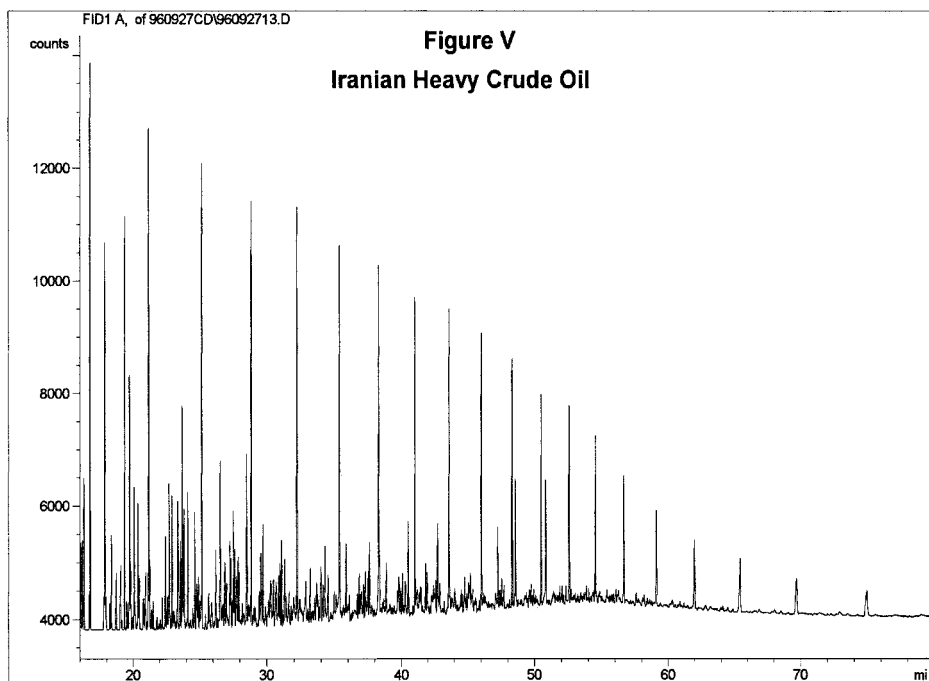
Annex 1.9 PASCAL Pattern Similarity Program Source Code

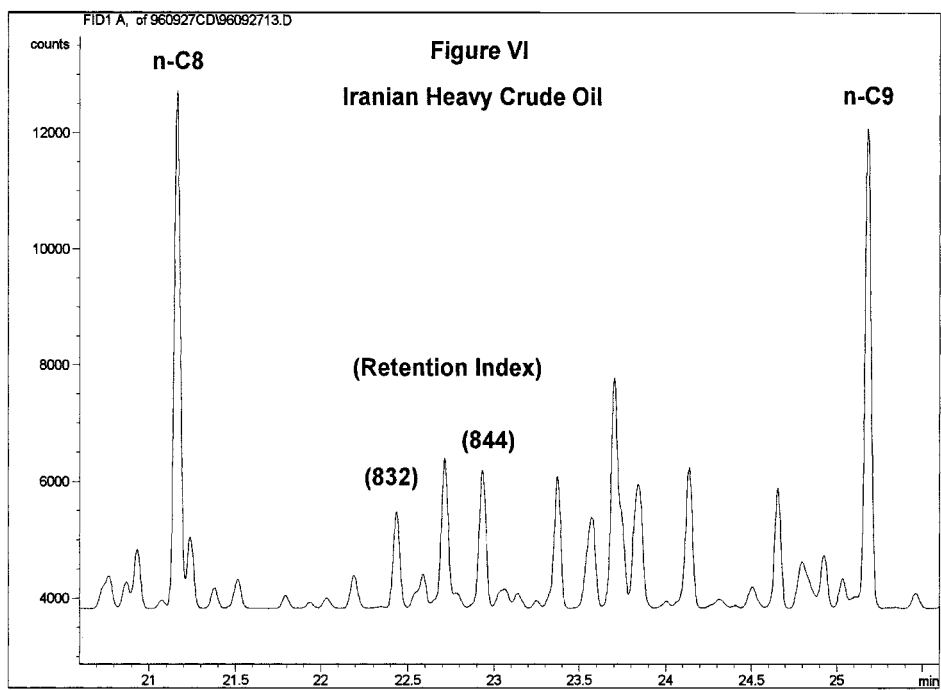


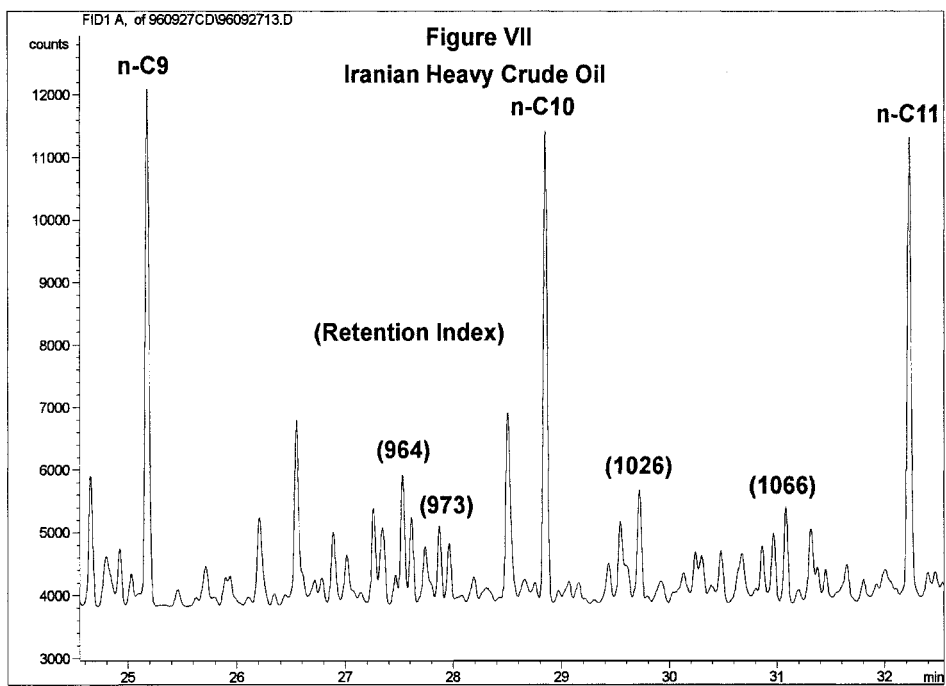


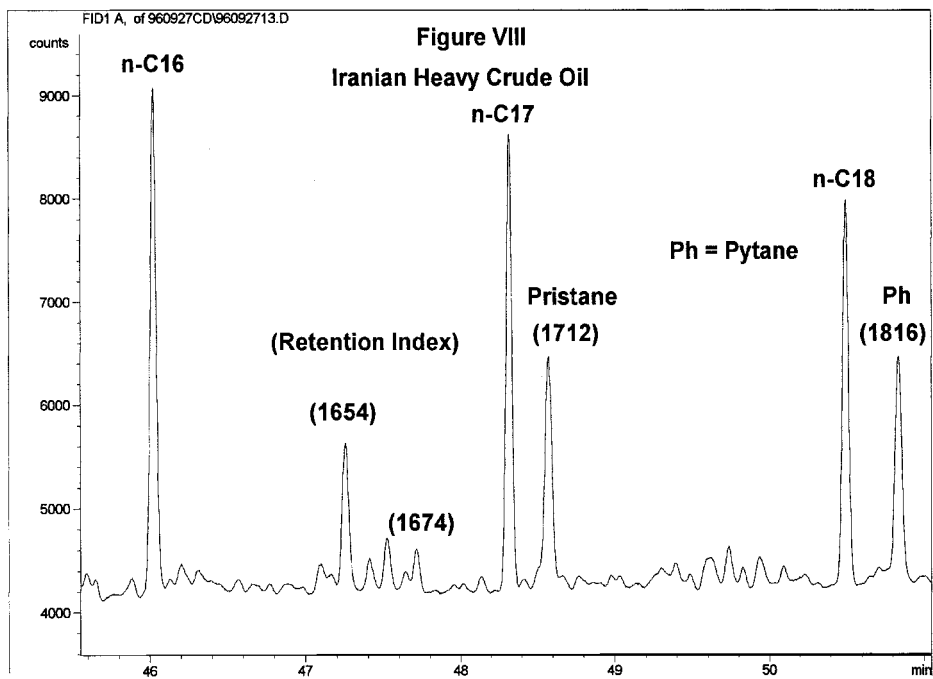












Annex 1 PASCAL Pattern Similarity Program (PPSP)

Annex **1.1** Directions on How to Use the PPSP

1.1.2 Directions on how to run the PASCAL Pattern Similarity Program (PPSP) using TURBO PASCAL version 4.0

All keyboard entries for this program are enclosed in curly brackets {}. If a return key is needed, CR is indicated after each entry. If the screen is cleared after an entry, cls is indicated. Responses from the computer are typed as they appear on the screen and are enclosed in [brackets]. Comments are enclosed in (parentheses).

1.1.3 The two example input data files, sample.txt and ref.txt, have been set-up and provided to the reader for the purpose of validating a local implementation of the PPSP program whose source code is supplied in **Annex 1.8**. The example sample input data file

is located in
Annex 1.3.
 The example
 reference
 input data file
 is located in
Annex 1.4.

1.1.4 The source code for
 this program as
 provided in **Annex 1.8**
 is configured to
 compile and run
 without modification
 from the C:\ drive.
 The C:\ drive must
 contain the following
 four items for this
 program to properly
 run:

- A. Turbo
Pascal
Versio
n 4.0
- B. This
progra
m,
PPSP.
PAS
- C. A
sample
input
data
file in
the
proper
format
- D. A
referen
ce
input
data
file in
the
proper
format

1.1.5 The same data format
 is used for both the
 sample data file and
 the reference data

file. Each data file is
 an ASCII text file with
 a precise definition of
 just what data go in
 which columns. The
 reference and sample
 data input files can be
 created by using any
 ASCII text editor or by
 using the integrated
 programming
 environment editor in
 Turbo Pascal. In the
 later case, type
 {turbo}CR at the C:\
 prompt and then {alt
 E} to access the text
 editor. When data
 entry is complete, the
 file is saved by
 pressing {F2} and
 providing a name for
 the file. The data
 format definition is as
 follows:

- A. Colum
ns
1-15 --
serial
no.
(e.g.
iraq_sa
mple_0
01)
- B. Colum
ns
16-21
-- run
no.
(e.g.
210792
)
- C. Next,
enter
the
retenti
on time
and
peak
area in
pairs,

s
e
p
a
r
a
t
i
n
g
e
a
c
h
e
n
t
r
y
b
y
a
s
p
a
c
e
a
s
t
h
i
s
i
s
a
s
p
a
c
e
d
e
l
i
m
i
t
e
d
f
o

r
m
a
t
s
c
h
e
m
e
-
-
(
e
. 9
. 2
2
. 8
7
3
1
2
2
3
. 3
9
3
2
7
4
9
. 0
0
2
9
9
8
5
1
. 2
6
3
8
0
0
-

1 -1).

D. Continue to enter the data into the same one line until the whole line (256 characters) is filled.

E. When the last entry has been entered, follow this by two negative numbers (e.g. 22.87 312 23.39 327 49.00 2998 51.26 3800 -1 -1) as this is a flag to indicate the last entry is reached.

F. In the sample

and reference data files, do not leave any blank spaces either before the first character space or after the last two characters, which are -1. When data entry is finished, press {F2} and the file name of your choice to save the file and leave the edit mode.

Annex

1.1.6

- A. If you are still in TURBO PASCAL, skip this step and proceed to **Annex 1.17**.
- B. If you are in MS-DOS and not in the C:\ directory, type

{CD
C:\}CR.
You
should
now be
at the
C:\
prompt
.

- C. At the C:\ prompt, type {turbo}CR to start Turbo Pascal.
- D. To load the program PPSP.PAS into the Turbo Pascal compiler, press {alt + F} and then {L}, and then at the input line the filename of the program {PPSP.PAS} followed by a CR.

the user to consider as possible responses.

- A. [Do you need instructions on how to prepare the input files?]
[Enter Y for yes and N for no.]
Enter {n}CR
- B. [Are the input files ready to be processed?]
[Enter Y for yes and N for no.]
Enter {y}CR
- C. [The input files are ready and program will continue.]
- D. [Enter the size of the window for the retention time.]
(The recommended size is between 0.05 to 0.1)
Enter {0.05}CR
- E. [The size of the window is 0.05]
- F. [Enter the number of the closest patterns you want to list.]
(The suggested

Annex 1.1.7 To compile and run the program PPSP.PAS press {alt + C} then {C} and then {CR} to compile the program and {Esc} to get back to the command portion of the Turbo Pascal compiler. The program is now ready to run.

Annex 1.1.8 To run the program, type {alt + R}. The program will start to run. The following instructions are suggested preliminary responses to questions that the program will ask the user. The entries here are only examples for

- values
are
between
n 10 to
30)
Enter {10}CR
[10 closest
patterns to the
sample pattern
will be listed.]
- G. [Enter the
name of the
sample file.]
(A copy of trial
sample data is
stored in
iraqsmp.txt)
Enter
{iraqsmp.txt}C
R
- H. [Enter the
name of the
reference file.]
(A copy of
trial reference
data is stored
in iraqref.txt)
Enter
{iraqref.txt}CR
- I. [Enter the
name of the
output file for
the summary.]
(A suggested
name is
c:\iraqres.txt)
Enter
{c:\iraqres.txt}C
R
- L. [Do you want
to store the
details of the
result?]
[Enter Y for
yes and N for
no.]
Enter {y}CR
- M. [Enter the
name of the
output file for
details.]
(A suggested
name is
c:\iraqdet.txt)
Enter
{c:\iraqdet.txt}
CR
- N. [>>>>iraq_sa
mple_001
210792<<<<<]
[Peak Number
1 22.87
312]
[Peak Number
2 23.39
327]
[Peak Number
3 49.00
2998]
[Peak Number
4 51.26
3800]

[Enter the
peak number
of the peak
you want to
normalize.]

Enter {1}CR
- O. [Peak 1
Retenti
on
Time
22.87
Peak
Area
312 is]
[chosen to be
normalized.]

[Program is
running....]

[The summary
is stored in the
file

c:\iraqr
es.txt]
[The details
are stored in
the file
c:\iraqdet.txt]

P. [Do you want
to continue
with another
set of data?]
[Enter Y for
yes or N for
no.]
Enter {n}CR

Q. [User does not
wish to
continue.]
[Program will
exit and return to Turbo Pascal.]

Annex 1.1.9 The program output results
are in a file on the C drive at
c:\iraqres.txt.

This file is an ASCII
text file that may be
read by any text
editor, the editor in
Turbo Pascal, or any
word processor.

Annex 1.1.10 The details of the program
output results are in a file on
the C drive at c:\iraqdet.txt.
This file is an ASCII text file
that may be read by any text
editor, the editor in Turbo
Pascal, or any word
processor.

Annex 1.2 Listing and Description of
Each Procedure in the PPSP

The name for each of
the 21 procedures
(**Annex 1.2.1** through
Annex 1.2.21) and
the main program
(**Annex 1.2.22**) of the
pattern recognition

program, PASCAL
Pattern Similarity
Program (PPSP), is
listed along with a
brief description. The
source code listing for
this Pascal program
consists of 1206 lines
of version 4.0 of
Turbo Pascal.
Following the listing of
the name of each
procedure is a pair of
numbers joined with a
dash listing the
beginning and ending
source code line
numbers for that
procedure. This is
followed by a brief
description of what
that procedure
accomplishes. An
asterisk (*) between
the number of the
procedure and the
name of the
procedure indicates
that the procedure is
one of the three
procedures (**Annex
1.2.12**, **Annex 1.2.15**,
and **Annex 1.2.20**)
and the main program
(**Annex 1.2.22**) whose
source code must be
modified when the
comparison metric is
changed.

Annex 1.2.1

CheckReal 61-93

This
procedure
checks to see
if the input
data is a real
number. If it is
not a real
number, the
program will
come back

		and ask the user for the data until the appropriate type of data has been entered.	Annex 1.2.4	CheckNoName141-159	The procedure checks to see if a name has been entered.
Annex 1.2.2	CheckInteger	94-123	Annex 1.2.5	CheckBlank	160-188
		This procedure checks to see if the input data is an integer. If it is not an integer, the program will come back and ask the user for the data until the appropriate type of data has been entered.			This procedure checks to see if there is a blank in the entered name, if so it will ask for the name to be entered again.
			Annex 1.2.6	CheckFile	189-235
					This procedure checks to see if the input file exists, if not, it will ask for it until it exists.
Annex 1.2.3	CheckSameName	124-140	Annex 1.2.7	CheckFileExist	236-294
		This procedure checks to see if the file name for the details of the calculations is the same as the file name for the summary of the calculations.			This procedure checks to see if the output file exists, if so, it asks if you want to write over it or provide the name of a new output file.
			Annex 1.2.8	CheckSummaryName	295-336
					This

		<p>procedure checks the name of the file entered by the user to store the summary of the calculations. If no name is entered, or the same name is entered, or the name has blanks, the user will be asked to enter the name again.</p>		<p>store the details of the calculations. If no name is entered, or the same name as the one for the summary, or the name has blanks, the user will be asked to enter the name again.</p>
			Annex 1.2.10	<p>Instruction 380-482</p> <p>This procedure provides instructions on how to set up the input files and asks, in separate questions, for the user to input the window retention time size and the number of closest references to list</p>
			Annex 1.2.11	<p>GetFiles 483-553</p> <p>This procedure asks, in separate questions, for the user to input the filename for the sample data file (an example is</p>
Annex 1.2.9	<p>CheckDetailName 337-379</p> <p>This procedure checks the name of the file entered by the user to</p>			

provided in **Annex 1.3)** which contains the sample input data, the filename for the reference data file (an example is provided in **Annex 1.4)** which contains the reference input data, the filename into which the program should put a summary of the program results, and the filename into which the program

should put the program details for the results. If no filename is provided for the details for the results, they will automatically be sent to the file junkfile.txt on the c:\ drive.

The Turbo Pascal Version 4.0 compiler, this program, the sample data file, and the reference data file must all be in the same directory on the computer. The output files will be created and placed into this directory automatically. This program is configured to operate in the C:\ directory

			without modific ation.		This procedure writes the reference input data for the reference samples to be compared from the reference data file (an example is provided in Annex 1.4) to the file specified in the procedure GetFiles (Annex 1.2.11). The similarity coefficient is also written.
Annex 1.2.12*	WriteResult	554- 610			
			This procedure writes a summary of the results of the pattern comparison into the file specified in the procedure GetFiles (Annex 1.2.11).	Annex 1.2.15*	WriteLongResult676-716
					This procedure writes the program details for the results of the comparison calculation into the output file as specified by the user in the procedure Getfiles (Annex 1.2.11).
Annex 1.2.13	WriteSample	611- 646			
			This procedure writes the sample input data for the sample to be compared from the sample data file (an example is provided in Annex 1.3) to the file specified in the procedure GetFiles (Annex 1.2.11).	Annex 1.2.16	GetData717-775
					This procedure reads into the program data from a data file.
				Annex 1.2.17	NormalizeSample776-827
					This procedure asks the user to choose the peak to be normalized to one and to input that peak number.
				Annex 1.2.18	GetRefPeak828-924
					This procedure picks out the peaks in the reference pattern that correspond to the peaks in the sample pattern so that the sample pattern can be compared to the reference pattern. The procedure to select the most appropriate reference peak is to find all reference peaks that are within the user supplied gas chromatographic
Annex	1.2.14	WriteRef	6 4 7 - 6 7 5		

-1074

This procedure enters the reference sample into the list of best reference samples in the ascending order of similarity coefficients.

Annex	1.2.19	NormalizeReference	9
			2
			5
			-
			9
			6
			1

This procedure will normalize the peaks in the reference set of data according to the peak chosen by the user for the sample set of data.

Annex	1.2.20*	GetCoefficient 9
		6
		2
		-
		9
		9
		2

This procedure computes two coefficients for each reference sample based upon two methods, the absolute difference distance and the Minkowski distance for $k = 2$, the classic Euclidean distance.

Annex	1.2.21	OrderArray	9 9 3
--------------	---------------	------------	-------------

Annex
1.2.22* Main Program1075-1206

This is the main program. It calls all of the preceeding procedures.

Annex

1.3 Example of a Sample Data File

iraq_sample_001210792 22.87 312 23.39 327
49 00 2998 51 26 3800 -1 -1

Annex

1.4 Example of a Reference Data File

```
iraq_sample_001210792 22.87 312 23.39 327
49.00 2998 51.26 3800 -1 -1
basl_reference1210758 23.17 495 23.69 503
49.19 4821 51.44 4769 -1 -1
kuwa_reference2210834 22.88 1365 23.39
944 49.00 1005 51.27 1393 -1 -1
irlt_reference3210166 22.43 1855 22.93 2348
48.58 2393 50.84 2615 -1 -1
irhv_reference4210168 22.43 1625 22.93
2362 48.58 2568 50.84 2585 -1 -1
```

Annex

1.5 Example of a Sample Results File

>>>>>>>>>>>>>>>SAMPLE<<<
<<<<<<<<<<<<<<<

SAMPLE Serial
Number: iraq_sample_001SAMPLE Run
Number: 210792

The Resolution is 1.00 and Peak 1 is chosen to be normalized.

>>Result of Absolute Difference Test<<

The Coefficient is 0.00 Serial no.:
iraq_sample_00
1
Run no.: 210792

The Coefficient is 2.71 Serial no.:
basl_reference1
Run no.: 210758

The Coefficient is 20.39 Serial no.:
kuwa_reference2
Run no.: 210168

The Coefficient is 20.65 Serial no.:
irhv_reference4
Run no.: 210166

The Coefficient is 20.70 Serial no.:
irlt_reference3
Run no.: 210166

>>Result of Minkowski Distance Test, k = 2<<

The Coefficient is 0.00 Serial no.:
iraq_sample_00
1
Run no.: 210792

The Coefficient is 2.55 Serial no.: basl_reference1
Run no.: 210758
The Coefficient is 14.02 Serial no.: irhv_reference4
Run no.: 210168
The Coefficient is 14.05 Serial no.: irlt_reference3
Run no.: 210166
The Coefficient is 14.26 Serial no.: kuwa_reference2
Run no.: 210834

Annex

1.6 Discussion and List of Alternate Minkowski Distance Parameters

In the general case, the absolute value Minkowski Distance, using the exponent k, is equal to the 1/k power of the sum, from n =1 to n, of the absolute value of the difference between the intensity (here, in units of either peak height or peak area) of each peak in the instant sample and the corresponding peak in the reference sample to the power of k. We use absolute values to maintain our conventional notion of distance as being greater than or equal to zero.

The use of Minkowski distance parameters, other than the two provided (k = 1, the absolute value of the difference distance and k = 2, the Euclidean distance), may be of assistance in two rare and extreme cases. The first case is where an instant sample and a set of reference samples are distinct, yet very similar. Essentially, as smaller fractional Minkowski distance parameters are used, the apparent scale expands, and it is easier to identify very small differences between an instant sample and a set of very similar reference samples. Minkowski distance parameters useful in this case are in the range of k = 0.1 to k = 0.5. The

second case is where an instant sample and a set of reference samples are clearly distinct and not at all similar. As larger Minkowski distance parameters are used, the apparent scale contracts, and it is easier to identify very large differences among very different reference samples. Minkowski distance parameters useful in this case are in the range of $k = 2.5$ to $k = 5.0$.

The PPSP source code provided in **Annex 1.8** as PPSP.PAS will directly compile as listed on the Turbo Pascal, Version 4.0, compiler from Borland International, Inc., copyright 1987.

Annex	1.7	List of Procedures Whose Source Code Must Be Modified To Enable PPSP to Use Different Minkowski Distance Parameters
		Three procedures (Annex 1.2.12 , Annex 1.2.15 , and Annex 1.2.20) and the Main Program (Annex 1.2.22) require source code modifications to enable Minkowski distances to be computed using alternate Minkowski distance parameters. The PPSP program source code listing provided in Annex 1.9 provides for the computation of two distance metrics for each reference sample, the absolute value of the difference distance (Minkowski distance parameter of $k = 1$) and the Euclidean distance (Minkowski distance parameter of $k = 2$).

Annex

1.9 PASCAL Pattern Similarity Program (PPSP.PAS) Source Code

```

{$R-}  {Range checking off}
{$B+}  {Boolean complete evaluation on}
{$S+}  {Stack checking on}
{$I+}  {I/O checking on}
{$N-}  {No numeric coprocessor}
{$M 65500,16384,655360} {Turbo 3 default
stack and heap}

PROGRAM
PASCAL_Pattern_Similarity_Program(INPU
T,OUTPUT);

{This program compares the GC pattern of
an unknown sample}
{with the GC patterns of some other known
samples.}
{The absolute difference between the peaks
and the Euclidean distance}
{are the two methods used to determine the
similarity of the patterns.}
{The sample data is stored in a file specified
by user and}
{the reference data in another file also
specified by user}
{The program reads in the sample data first.}
{Then it reads in the reference data one at a
time.}
{The user can choose whichever peak he
wants to normalize against.}
{A lower value in the absolute difference or
the Euclidean distance}
{will indicate the patterns are more similar.}
{The summary of results are recorded in an
output file given by user.}

CONST
  MaxPeak = 50;
  MaxArray = 40;

```

Annex	1.8	Pascal Compiler Requirements
--------------	------------	------------------------------

```

TYPE
  String15 = STRING[15];
  String14 = STRING[15];
  String13 = STRING[13];
  String6 = STRING[6];
  GcPattern = RECORD
    SerialNo : String15;
    RunNo : String6;
    Time : ARRAY [1..MaxPeak] OF
REAL;
    Peak : ARRAY [1..MaxPeak] OF
REAL;
    NumPeak : INTEGER;
    Coeff : REAL
  END;
  ArrayOfPattern = ARRAY [1..MaxArray] OF
GcPattern;
  MatchType = ARRAY [1..MaxPeak] OF
BOOLEAN;

VAR
  Reference,Sample,NormSample,RefSelect
: GcPattern;
  GoodRef1,GoodRef2 : ArrayOfPattern;
  RefFile,SmpFile,Result,LongResult : TEXT;
  RefName,SmpName,Summary,Details :
String14;
  Match : MatchType;

Ready,Overflow,BadData,RefOK,NoDetail,C
ontinue : BOOLEAN;
  Resolution,Coeff1,Coeff2 : REAL;
  Best,NormPeak,Count1,Count2,index :
INTEGER;
  Answer : CHAR;

```

```

PROCEDURE CheckReal (VAR InData :
REAL;
                     VAR IO : INTEGER);

```

```

{This procedure checks if the typed-in data
is a real number.}
{If it is not, then there will be an I/O error and
the program will bomb.}
{This procedure will prevent the program
from bombing from bad input data.}
{Instead, it will come back to ask for the data
once more}
{until the appropriate type has been

```

```

entered.}

```

```

VAR
  GoodData : BOOLEAN;

```

```

BEGIN

```

```

  GoodData := FALSE;
  WHILE NOT GoodData DO
    BEGIN
      WRITELN;
      WRITELN('Bad Data. Enter the number
again. ');
      {$I-} READLN(InData); {$I+}
      IO := IOResult;
      {! 1. IOResult now returns different values
corresponding to DOS error codes.}
      IF (IO<>0) OR (InData<=0.0) THEN
        GoodData := FALSE
      ELSE GoodData := TRUE
    END
  END;

```

```

END;

```

```

PROCEDURE CheckInteger (VAR InData, IO
: INTEGER);

```

```

{This procedure checks if the input data is
an integer.}
{If not, it prevents the program from
bombing}
{but keeping requesting for more until the
input is an integer.}

```

```

VAR
  GoodData : BOOLEAN;

```

```

BEGIN

```

```

  GoodData := FALSE;
  WHILE NOT GoodData DO
    BEGIN
      WRITELN;
      WRITELN('Bad Data. Enter the number
again. ');
      {$I-} READLN(InData); {$I+}

```

```

        IO := IOResult;
    {! 2. IOResult now returns different values
    corresponding to DOS error codes.}
    IF (IO<>0) OR (Indata<=0) THEN
        GoodData := FALSE
    ELSE GoodData := TRUE
    END
END;

```

```

PROCEDURE CheckSameName(VAR
    InName : String14;
                        ExistName : String14;
                        VAR SameName :
BOOLEAN);

```

```

{This procedure checks if the name for
details is the same as}
{the one for summary. If this is so,
SameName is true.}

```

```

BEGIN

```

```

    SameName := FALSE;
    IF InName = ExistName THEN SameName
:= TRUE

```

```

END;

```

```

PROCEDURE CheckNoName (Filename :
String14;
                        VAR NoName : BOOLEAN);

```

```

{This procedure checks if a name has been
entered.}
{If not, NoName will be true.}

```

```

VAR
    LengthOfName : INTEGER;

```

```

BEGIN
    LengthOfName := LENGTH(Filename);
    IF LengthOfName <= 0 THEN NoName :=
TRUE

```

```

    ELSE NoName := FALSE
END;

```

```

PROCEDURE CheckBlank (Filename :
String14;
                        VAR HasBlank : BOOLEAN);

```

```

{This procedure checks if there is any blank
in the name entered.}
{If there is any, the program will flag this as
a mistake.}
{The user will then asked to enter the name
again.}

```

```

CONST
    Blank = ' ';

```

```

VAR
    i, LengthOfName : INTEGER;

```

```

BEGIN
    LengthOfName := LENGTH(Filename);
    i := 0;
    HasBlank := FALSE;
    REPEAT
        i := i+1;
        IF Filename[i] = Blank THEN HasBlank :=
TRUE
    UNTIL HasBlank OR (i>=LengthOfName)

```

```

END;

```

```

PROCEDURE CheckFile (VAR Infile : TEXT;
                        VAR Filename : String14;
                        ExistName : String14;
                        VAR IO : INTEGER);

```

```

{This procedure checks if the input file
exists.}
{If it doesn't, the procedure will prevent the
program from bombing.}
{Instead, it will ask for the filename again
until one exists.}

```

```
VAR
  GoodData, SameName, NoName, HasBlank
: BOOLEAN;
```

```
BEGIN
```

```
  SameName := FALSE;
  NoName := FALSE;
  HasBlank := FALSE;
  GoodData := FALSE;
  WHILE NOT GoodData DO
    BEGIN
      CheckNoName(Filename, NoName);
      IF Not NoName THEN
        CheckBlank(Filename, HasBlank);
      IF (Not NoName) AND (Not HasBlank)
      THEN
        CheckSameName(Filename, Existname,
          SameName);
      IF (IO<>0) OR NoName OR HasBlank
      OR SameName THEN
        GoodData := FALSE
      ELSE GoodData := TRUE;
      IF Not GoodData THEN
        BEGIN
          WRITELN;
          IF SameName THEN
            WRITELN('Same name as sample
file. Enter another name for reference file.')
          ELSE WRITELN('Input file does not
exist. Enter the filename again. ');
          READLN(Filename);
          ASSIGN(Infile, Filename);
          {$I-} RESET(Infile); {$I+}
          IO := IOResult
        {! 3. IOResult now returns different values
        corresponding to DOS error codes.}
        END
      END
    END
```

```
END;
```

```
PROCEDURE CheckFileExist (VAR
  Filename : String14;
  VAR OK : BOOLEAN);
```

```
{This procedure checks if the name of the
output file already exists.}
{If so, then FileExist will be true.}
```

```
{The program will inform the user that file
already exists.}
{The user may decide to write over the
existing file.}
{If not, the program will ask the user to enter
another name for the output file.}
```

```
VAR
  DummyFile : TEXT;
  IO : INTEGER;
  FileExist : BOOLEAN;
```

```
BEGIN
```

```
  OK := TRUE;
  FileExist := FALSE;
  ASSIGN(DummyFile, Filename);
  {$I-} RESET(DummyFile); {$I+}
  IO := IOResult;
  {! 4. IO^Result now returns different values
  corresponding to DOS error codes.}
  IF IO = 0 THEN
    BEGIN
      FileExist := TRUE;
      WRITELN;
      WRITELN('Output file already exists.
Enter Y to write over the file. ');
      READLN(Answer);
      IF Answer IN ['y', 'Y'] THEN OK := TRUE
    ELSE
      BEGIN
        OK := FALSE;
        WRITELN('User does not wish to
write over existing file. ');
        WRITELN('Enter another name for the
output file. ');
        READLN(Filename)
      END
    END
  ELSE
    BEGIN
      {$I-} REWRITE(DummyFile); {$I+}
      IO := IOResult;
      {! 5. IOResult now returns different values
      corresponding to DOS error codes.}
      IF IO <> 0 THEN
        BEGIN
          WRITELN;
          WRITELN('Bad Name. Enter again. ');
          READLN(Filename);
          OK := FALSE
        END
      END
```

```

    END;
    {$I-} CLOSE(DummyFile); {I+}
    IO := IOResult;
    {! 6. IO^Result now returns different values
    corresponding to DOS error codes.}
    IF IO <> 0 THEN OK := FALSE

```

```

END;

```

```

PROCEDURE CheckSummaryName (VAR
Summary : String14;
                        SmpName,RefName :
String14);

```

```

{This procedure checks the name of the file
entered by user.}
{If no name is entered or there are blanks in
the name,}
{the program will flag this as a mistake.}
{The user will be asked to enter the name
again.}

```

```

VAR
    SameName,NoName,HasBlank,OK :
BOOLEAN;
    Answer : CHAR;

```

```

BEGIN

```

```

    SameName := TRUE;
    NoName := TRUE;
    HasBlank := TRUE;
    OK := TRUE;
    REPEAT
        WHILE NoName OR HasBlank OR
SameName DO
            BEGIN

```

```

                CheckSameName(Summary,SmpName,Sa
meName);
                IF NOT SameName THEN
                CheckSameName(Summary,RefName,Sam
eName);
                IF NOT SameName THEN
                CheckNoName(Summary,NoName);
                IF (NOT NoName) AND (NOT
SameName) THEN
                CheckBlank(Summary,HasBlank);

```

```

                IF NoName OR HasBlank OR
SameName THEN
                    BEGIN
                        WRITELN;
                        WRITELN('Bad name. Enter the
filename again. ');
                        READLN(Summary)
                    END
                END;
                CheckFileExist(Summary,OK);
                IF NOT OK THEN NoName := TRUE
{Make sure new name is checked again}
                UNTIL OK;

```

```

END;

```

```

PROCEDURE CheckDetailName (VAR
Details : String14;

```

```

Summary,SmpName,RefName : String14);

```

```

{This procedure checks the name given to
store the details.}
{If no name is given, or there is blanks in the
name, or}
{if the name is the same as the one for the
summary.}
{If this is so, the program will flag this as a
mistake and}
{the user will be asked to enter the name
again.}

```

```

VAR
    SameName,NoName,HasBlank,OK :
BOOLEAN;

```

```

BEGIN

```

```

    SameName := TRUE;
    NoName := TRUE;
    HasBlank := TRUE;
    OK := TRUE;
    REPEAT
        WHILE NoName OR HasBlank OR
SameName DO
            BEGIN

```

```

                CheckSameName(Details,Summary,SameN

```

```

ame);
    IF NOT SameName THEN
CheckSameName(Details,RefName,SameName);
ame);
    IF NOT SameName THEN
CheckSameName(Details,SmpName,SameName);
    IF NOT SameName THEN
CheckNoName(Details,NoName);
    IF (NOT NoName) AND (NOT SameName) THEN
CheckBlank(Details,HasBlank);
    IF NoName OR HasBlank OR SameName THEN
        BEGIN
            WRITELN;
            WRITELN('Bad Name. Enter the filename again. ');
            READLN(Details)
        END
    END;
    CheckFileExist(Details,OK);
    IF NOT OK THEN NoName := TRUE
{Allow new name to be checked again.}
    UNTIL OK

END;

```

```

PROCEDURE Instruction (VAR Ready :
BOOLEAN;

```

```

    VAR Resolution : REAL;
    VAR Best : INTEGER);

```

```

{This procedure gives the instructions on
how to set up input files.}
{If the input files are not ready yet, the
program will terminate.}
{Otherwise, the user will give the size of the
window for the retention time}
{and the number of closest references he
would like to list.}

```

```

VAR
    Answer : CHAR;
    IO : INTEGER;

```

```

BEGIN

```

```

    WRITELN;

```

```

    WRITELN('Do you need instructions on
how to prepare the input files?');
    READLN(Answer);
    WRITELN;
    IF Answer IN ['Y','y'] THEN
        BEGIN
            WRITELN('Before this program can be
run, two input files need to be set up:');
            WRITELN(' one for sample data and
one for reference data. ');
            WRITELN;
            WRITELN('The format for the data in
both files are the same:');
            WRITELN;
            WRITELN('** columns 1-15 -- serial no.
(e.g. iraq_sample_001)');
            WRITELN;
            WRITELN('** columns 16-21 -- run no.
(e.g. 210792)');
            WRITELN;
            WRITELN('** next, enter the retention
time and peak area in pairs,');
            WRITELN(' separating each entry by a
space. ');
            WRITELN(' (e.g. 22.87 312 23.39 327
49.00 2998 51.26 3800 -1 -1)');
            WRITELN;
            WRITELN('** continue enter the data in
one line');
            WRITELN(' until the whole line (256
characters) is filled. ');
            WRITELN;
            WRITELN('** when the last entry has
been entered,');
            WRITELN(' follow this by two negative
numbers. ');
            WRITELN(' (e.g. 22.87 312 23.39 327
49.00 2998 51.26 3800 -1 -1)');
            WRITELN(' this is a flag to indicate the
last entry is reached. ');
            WRITELN
        END;

```

```

    WRITELN('Are the input files ready to be
processed?');
    WRITELN('Enter Y for yes and N for no. ');
    READLN(Answer);
    WRITELN;
    IF Answer IN ['Y','y'] THEN
        BEGIN
            Ready := TRUE;
            WRITELN('The input files are ready

```

```

and program will continue. ');
    WRITELN
    END
ELSE
    BEGIN
        Ready := FALSE;
        WRITELN('Input files are not ready to
be processed. ');
        WRITELN('Refer to the REFERENCE
GUIDE on how to set up files. ');
        WRITELN
    END;

    IF Ready THEN
        BEGIN
            Resolution := -1.0;
            WRITELN;
            WRITELN('Enter the size of the window
for the retention time. ');
            WRITELN('The recommended size is
between 0.05 to 0.1 ');
            {$I-} READLN(Resolution); {$I+}
            IO := IOResult;
            {! 7. IOResult^ now returns different values
            corresponding to DOS error codes.}
            IF (IO<>0) OR (Resolution<=0.0) THEN
                CheckReal(Resolution,IO);
                WRITELN;
                WRITELN('The size of the window is
',Resolution:5:2);
                WRITELN;

                Best := -1;
                WRITELN;
                WRITELN('Enter the number of the
closest patterns you want to list. ');
                WRITELN('The suggested values are
between 10 to 30 ');
                {$I-} READLN(Best); {$I+}
                IO := IOResult;
                {! 8. IOResult^ now returns different values
                corresponding to DOS error codes.}
                IF (IO<>0) OR (Best<=0) THEN
                    CheckInteger(Best,IO);
                    IF Best > MaxArray THEN
                        REPEAT
                            WRITELN('The number you entered
exceeds the allocations space which is
',MaxArray:3);
                            WRITELN('Enter another number
which is smaller than ',MaxArray:3);
                            {$I-} READLN(Best); {$I+}

```

```

            IO := IOResult;
            {! 9. IOResult now^ returns different values
            corresponding to DOS error codes.}
            IF IO <> 0 THEN
                CheckInteger(Best,IO);
                UNTIL Best <= MaxArray;
                WRITELN;
                WRITELN(Output,Best:3,' closest
patterns to the sample pattern will be
listed. ');
                WRITELN
            END

```

```

END;

```

```

PROCEDURE GetFiles (VAR
SmpFile,RefFile,Result,LongResult : TEXT;
    VAR
SmpName,RefName,Summary,Details :
String14;
    VAR NoDetail : BOOLEAN);

```

```

{This procedure reads in the names of the
input files and output files.}
{The two input files are sample file and
reference file.}
{The two output files are one for
summarization of results and one for
details.}
{The user may choose not to include the
details for saving space.}

```

```

VAR
    Answer : CHAR;
    IO : INTEGER;

```

```

BEGIN

```

```

    WRITELN;
    WRITELN('Enter the name of the sample
file. ');
    WRITELN('(A copy of trial sample data is
stored in iraqsmpt.txt) ');
    READLN(SmpName);
    ASSIGN(SmpFile,SmpName);
    {$I-} RESET(SmpFile); {$I+}
    IO := IOResult;
    {! 10. IOResult now returns different values

```



```

BEGIN

  WITH Indata DO
    BEGIN
      WRITE(Result,'The coefficient is
',Coeff:6:2);
      WRITELN(Result,'  Serial no.:
',SerialNo,'  Run no.: ',RunNo);
      FOR i := 1 TO NumPeak DO

WRITELN(Result,Time[i]:6:2,Peak[i]:12:4);
      WRITELN(Result)
    END

  END;

```

```

PROCEDURE WriteLongResult (VAR
LongResult : TEXT;
                          Sample, NormSample :
GcPattern;
                          GoodRef1, GoodRef2 :
ArrayOfPattern;
                          Resolution : REAL;
                          NormPeak, Count1, Count2
: INTEGER);

```

```

{This procedure writes the details of the
results to the output file}
{whose name is given by the user.}
{The output data include the serial number,
the run number,}
{the retention time, the normalized peak
area and the coefficient.}
{The references are listed in the ascending
order of the coefficients.}

```

```

VAR
  i : INTEGER;

```

```

BEGIN

```

```

  IF Count1 > Best THEN Count1 := Best;
  IF Count2 > Best THEN Count2 := Best;
  WRITELN (LongResult);
  WRITELN (LongResult);
  WriteSample
(LongResult, Sample, Resolution, NormPeak);
  WriteRef (LongResult, NormSample);

```

```

  WRITELN (LongResult);
  WRITELN (LongResult,'>>Result of
Euclidean Distance Test<<');
  WRITELN (LongResult);
  FOR i := 1 TO Count1 DO
    WriteRef (LongResult, GoodRef1[i]);
  WRITELN (LongResult);
  WRITELN (LongResult,'>>Result of
Euclidean Distance Test<<');
  WRITELN (LongResult);
  FOR i := 1 TO Count2 DO
    WriteRef (LongResult, GoodRef2[i]);
  WRITELN (LongResult);

```

```

END;

```

```

PROCEDURE GetData (MaxPeak :
INTEGER;
                  VAR Infile : TEXT;
                  VAR Indata : GcPattern;
                  VAR Overflow : BOOLEAN;
                  VAR BadData : BOOLEAN);

```

```

{This procedure reads the data from the
data file one at a time.}
{Each set of data consists of serial no., run
no., retention time}
{and peak area for each peak.}
{The procedure will indicate if there is not
enough space to read}
{all the data in the variable Overflow.}

```

```

VAR
  i, IO : INTEGER;

```

```

BEGIN

```

```

  WITH Indata DO
    BEGIN
      READ(Infile, SerialNo, RunNo);
      i := 0;
      REPEAT
        i := i+1;
        {$I-} READ(Infile, Time[i], Peak[i]); {$I+}
        IO := IOResult;
        {! 12. IOResult now returns different values
        corresponding to DOS error codes.}
        IF IO <> 0 THEN

```

```

        BEGIN
            WRITELN;
            WRITELN('Bad Data in the Input
File');
            WRITELN('Program will terminate for
this set of data. ');
            WRITELN;
            BadData := TRUE
        END;
        UNTIL (Time[i]<0.0) OR (i>=MaxPeak)
OR BadData;
        IF NOT BadData THEN
            BEGIN
                IF Time[i] < 0.0 THEN
                    NumPeak := i - 1
                ELSE
                    BEGIN
                        WRITELN;
                        WRITELN('>>>>>ARRAY
OVERFLOW<<<<<');
                        WRITELN('SerialNo, ' ',RunNo,' has
more data than the space allocated. ');
                        WRITELN('The dimension of the
array is given by MaxPeak whose present
value is ',MaxPeak:3);
                        WRITELN('The program will
terminate for this set of data. ');
                        WRITELN;
                        Overflow := TRUE
                    END
                END
            END;
            READLN(Infile)
        END;

```

```

PROCEDURE NormalizeSample (Sample :
GcPattern;
                        VAR NormSample :
GcPattern;
                        VAR NormPeak :
INTEGER);

```

{This procedure allows the user to choose one of the peaks}
{in the sample pattern to be normalized to one.}

VAR

i,IO : INTEGER;

```

BEGIN
    WITH Sample DO
        BEGIN
            WRITELN;
            WRITELN('>>>>>',SerialNo,'
',RunNo,'<<<<<');
            FOR i := 1 TO NumPeak DO
                WRITELN('Peak Number
',i:3,Time[i]:10:2,Peak[i]:10:0);
                REPEAT
                    NormPeak := 0;
                    WRITELN('Enter the peak number of
the peak you want to normalize. ');
                    {$I-} READLN(NormPeak); {$I+}
                    IO := IOResult;
                    {! 13. IOResult now returns different values
corresponding to DOS error codes.}
                    IF (NormPeak<=0) OR
(NormPeak>NumPeak) THEN IO := 10;
                    WHILE IO <> 0 DO
                        BEGIN
                            CheckInteger(NormPeak,IO);
                            IF NormPeak > NumPeak THEN IO
:= 10
                        END;
                        UNTIL Peak[NormPeak] > 0.0;
                        WRITELN;
                        WRITE('Peak ',NormPeak:3,' Retention
Time ',Time[NormPeak]:6:2,' Peak Area
',Peak[NormPeak]:6:0);
                        WRITELN(' is chosen to be
normalized. ');
                        WRITELN('Program is running.... ');
                        WRITELN;
                        NormSample.SerialNo := SerialNo;
                        NormSample.RunNo := RunNo;
                        FOR i := 1 TO NumPeak DO
                            BEGIN
                                NormSample.Time[i] := Time[i];
                                NormSample.Peak[i] :=
Peak[i]/Peak[NormPeak]
                            END;
                                NormSample.NumPeak := NumPeak
                        END
                    END;
                END;
            END;

```

```

PROCEDURE GetRefPeak
(Reference, Sample : GcPattern;
  Resolution : REAL;
  NormPeak : INTEGER;
  VAR RefSelect : GcPattern;
  VAR Match : MatchType;
  VAR RefOK : BOOLEAN);

{This procedure picks out the corresponding
peaks in the reference pattern}
{so that the sample pattern can be
compared to it.}
{The procedure to match the peaks is as
follows:}
{ 1. Find the peaks that are within the
resolution.}
{ 2. Pick the one with the smallest time
differences.}
{ 3. Store this matching peak under the
variable RefSelect.}
{If a peak cannot be matched, the indicator
Match will be FALSE.}

VAR
  TimeDiff1, TimeDiff2 : REAL;
  i, j, k : INTEGER;
  SmallerDiff : BOOLEAN;

BEGIN

{Initialize variables}

FILLCHAR(RefSelect, SIZEOF(RefSelect), C
HR(0));
FOR i := 1 TO MaxPeak DO
  Match[i] := FALSE;
  j := 0;
  k := 0;

  RefSelect.SerialNo := Reference.SerialNo;
  RefSelect.RunNo := Reference.RunNo;

  WITH Sample DO
    BEGIN
      FOR i := 1 TO NumPeak DO
        BEGIN
          {Set j to the peak that is last picked}
          j := k;
          {Pick first peak that falls within the
resolution}

```

```

REPEAT
  Match[i] := FALSE;
  j := j+1;
  TimeDiff1 := Reference.Time[j] -
Time[i];
  TimeDiff1 := ABS(TimeDiff1);
  IF TimeDiff1 <= Resolution THEN
    Match[i] := TRUE
  UNTIL Match[i] OR
(j>=Reference.NumPeak);

{Next, pick peak with smallest time
difference within resolution}
IF Match[i] THEN
  BEGIN
    k := j;
    SmallerDiff := TRUE;
    WHILE (j<Reference.NumPeak)
AND SmallerDiff DO
      BEGIN
        j := j+1;
        TimeDiff2 := Reference.Time[j] -
Time[i];
        TimeDiff2 := ABS(TimeDiff2);
        IF TimeDiff2 < TimeDiff1 THEN
          BEGIN
            SmallerDiff := TRUE;
            TimeDiff1 := TimeDiff2;
            k := j
          END
        ELSE
          SmallerDiff := FALSE
        END;

      {Put matching peak in RefSelect}
      RefSelect.Time[i] :=
Reference.Time[k];
      RefSelect.Peak[i] :=
Reference.Peak[k];
      RefSelect.NumPeak :=
RefSelect.NumPeak + 1;
      Reference.Time[k] := 0.0
    END

    {When no match, set peak area to zero for
that retention time}
    ELSE
      BEGIN
        RefSelect.Time[i] := Time[i];
        RefSelect.Peak[i] := 0.0;
        RefSelect.NumPeak :=
RefSelect.NumPeak + 1
      END

```

```

        END

    END;

    {If peak to be normalized is zero, reference
    is automatically discarded}
    {as indicated by the variable RefOK}
    IF Match[NormPeak] = TRUE THEN
        RefOK := TRUE
    ELSE RefOK := FALSE

END;

PROCEDURE NormalizeReference
(NormPeak : INTEGER;
    Match : MatchType;
    VAR RefSelect :
GcPattern;
    VAR RefOK :
BOOLEAN);

{This procedure will normalize the peaks in
the reference}
{according to the peak chosen by the user for
the sample.}
{If there is no corresponding peak, reference
is considered not similar}
{and its coefficient is not computed at all.}

VAR
    i : INTEGER;
    NormValue : REAL;

BEGIN

    WITH RefSelect DO
        BEGIN

            NormValue := Peak[NormPeak];
            IF Match[NormPeak] AND
(Peak[NormPeak]>0.0) THEN
                BEGIN
                    RefOk := TRUE;
                    FOR i := 1 TO NumPeak DO
                        Peak[i] := Peak[i]/NormValue
                    END
                ELSE
                    RefOk := FALSE

```

```

        END

    END;

    PROCEDURE GetCoefficient
    (NormSample,RefSelect : GcPattern;
        VAR Coeff1,Coeff2 :
    REAL);

    {This procedure will compute two
    coefficients for each reference}
    {based on two methods.}
    {The first one is to take the absolute
    difference of the peak area}
    {between the sample and the reference.}
    {The second one is the Euclidean distance,
    that is}
    {the square root of the sum of the squares of
    the difference.}
    {In this way we can compare the two
    methods.}

    VAR
        i : INTEGER;

    BEGIN

        Coeff1 := 0.0;
        Coeff2 := 0.0;
        FOR i := 1 TO NormSample.NumPeak DO
            BEGIN
                Coeff1 := Coeff1 +
ABS(NormSample.Peak[i] -
RefSelect.Peak[i]);
                Coeff2 := Coeff2 +
SQR(NormSample.Peak[i] -
RefSelect.Peak[i])
            END;
            Coeff2 := SQRT(Coeff2)

        END;

    PROCEDURE OrderArray (RefSelect :
GcPattern;
        Coefficient : REAL;
        VAR GoodRef :

```



```
FILLCHAR(Reference,SIZEOF(Reference),CHR(0));
```

```
FILLCHAR(Sample,SIZEOF(Sample),CHR(0));
```

```
FILLCHAR(NormSample,SIZEOF(NormSample),CHR(0));
```

```
FILLCHAR(RefSelect,SIZEOF(RefSelect),CHR(0));
```

```
FILLCHAR(GoodRef1,SIZEOF(GoodRef1),CHR(0));
```

```
FILLCHAR(GoodRef2,SIZEOF(GoodRef2),CHR(0));
```

```
FILLCHAR(Match,SIZEOF(Match),CHR(0));  
Ready := TRUE;  
Overflow := FALSE;  
BadData := FALSE;  
RefOK := TRUE;  
Continue := TRUE;  
Resolution := 0.1;  
NormPeak := 1;  
Count1 := 0;  
Count2 := 0;  
Coeff1 := 0.0;  
Coeff2 := 0.0;  
{End of Initialization}
```

```
WHILE Continue DO  
BEGIN  
Instruction(Ready,Resolution,Best);  
IF Ready THEN  
BEGIN  
{Open the input files containing sample data  
and reference data}  
{and the output files to store the results of  
this program}
```

```
GetFiles(SmpFile,RefFile,Result,LongResult,  
SmpName,RefName,Summary,Details,NoDe  
tail);
```

```
{Compare each set of sample to the list of  
references}
```

```
REPEAT  
FOR index := 1 TO Best DO  
BEGIN
```

```
FILLCHAR(GoodRef1,SIZEOF(GoodRef1),CHR(0));
```

```
FILLCHAR(GoodRef2,SIZEOF(GoodRef2),CHR(0));
```

```
END;  
Overflow := FALSE;  
BadData := FALSE;  
{Reads in sample data one set at a time}
```

```
GetData(MaxPeak,SmpFile,Sample,Overflow,  
BadData);
```

```
IF (NOT Overflow) AND (NOT  
BadData) THEN  
BEGIN  
{Normalize the peaks of the sample data}
```

```
NormalizeSample(Sample,NormSample,NormPeak);  
{Count1 keeps track of best references for  
absolute difference method}  
{Count2 keeps track of best references for  
euclidean distance method}  
Count1 := 0;  
Count2 := 0;
```

```
{Compare each reference to sample,  
compute the 2 coefficients according to}  
{the two methods used: absolute difference  
and euclidean distance}  
{Then place the reference on the best  
references list accordingly.}
```

```
WHILE NOT EOF(RefFile) AND  
(NOT Overflow) AND (NOT BadData) DO  
BEGIN  
Overflow := FALSE;  
BadData := FALSE;
```

```
GetData(MaxPeak,RefFile,Reference,Overflow,  
BadData);
```

```
IF (NOT Overflow) AND (NOT  
BadData) THEN  
BEGIN  
{Get the matching peaks in the reference}
```

```
GetRefPeak(Reference,NormSample,Resolution,  
NormPeak,RefSelect,Match,RefOK);  
{If the peak to be normalized to one has zero  
area, then reference is}  
{automatically discarded. RefOK is then set  
to false.}
```

```
IF RefOK THEN
```

```

        BEGIN
{Normalize the peaks of the reference}

NormalizeReference(NormPeak,Match,RefS
elect,RefOK);
        IF RefOK THEN
            BEGIN
{Compute the 2 coefficients according to the
two methods used:}
{ absolute difference and euclidean
distance}

GetCoefficient(NormSample,RefSelect,Coeff
1,Coeff2);
{Place the best references in the two lists:
GoodRef1, GoodRef2}
{The best references will be listed in the
ascending order of the coefficients.}

OrderArray(RefSelect,Coeff1,GoodRef1,Cou
nt1);

OrderArray(RefSelect,Coeff2,GoodRef2,Cou
nt2)

            END
        END
    END
END;

        CLOSE(RefFile);
{Write the summary of the results to the
output file on the diskette}
        WriteResult
(Result,Sample,GoodRef1,GoodRef2,Resolu
tion,NormPeak,Count1,Count2);
        IF NOT NoDetail THEN
{Write the details of the results to another
output file on the diskette}
        WriteLongResult
(LongResult,Sample,NormSample,GoodRef
1,GoodRef2,Resolution,NormPeak,Count1,C
ount2);
{Reset the reference file to compare another
set of sample data}
        ASSIGN(RefFile,RefName);
        RESET(RefFile)
    END
    UNTIL EOF(SmpFile) OR Overflow
OR BadData;

        CLOSE(SmpFile);
        CLOSE(Result);

```

```

        CLOSE(LongResult)
    END;
    IF (NOT Overflow) AND (NOT BadData)
    THEN
        BEGIN
            WRITELN;
            WRITELN('The summary is stored in
the file ',Summary);
            IF NOT NoDetail THEN
                WRITELN('The details is stored in the
file ',Details);
            WRITELN
            END;
            WRITELN;
            WRITELN('Do you want to continue with
another set of data?');
            WRITELN('Enter Y for yes and N for
no. ');
            READLN(Answer);
            IF Answer IN ['Y','y'] THEN Continue :=
TRUE
            ELSE
                BEGIN
                    Continue := FALSE;
                    WRITELN;
                    WRITELN('User does not wish to
continue. ');
                    WRITELN('Program will exit and
return to Turbo Pascal. ');
                    WRITELN
                END
            END;

        END;

    END.

{      END OF PROGRAM      }

```